analytical chemistry

4/76
V.



# Mass Spectrometry

**A. L. Burlingame and B. J. Kimble**

*Space Sciences Laboratory, University of California, Berkeley, Calif. 94720*

**Peter J. Derrick**

*Department of Physical Chemistry, La Trobe University, Bundoora, Melbourne 3083, Australia*

**Volume 48, Number 5**

**Pages 368R–403R, April 1976**

Reprinted from ANALYTICAL CHEMISTRY ANNUAL REVIEWS, Vol. 48, Page 368R, April 1976


# Mass Spectrometry

**A. L. Burlingame* and B. J. Kimble**

*Space Sciences Laboratory, University of California, Berkeley, Calif. 94720*

**Peter J. Derrick**

*Department of Physical Chemistry, La Trobe University, Bundoora, Melbourne 3083, Australia*

## OVERVIEW

The multifarious interests and pursuits covered by the name "mass spectrometry" all but deny definition of the scope or the focal point of this encompassing but divergent suite of scientific subjects. Perhaps the physical chemistry and the instrumentation with its analytical power once provided some sort of central ground clearly visible from all corners of the then fledgling field, but it is doubtful whether this is now true considering the present extent of the empire. Significant analytical contributions are emanating from medical and environmental laboratories with relatively little previous interest in mass spectrometry and perhaps no more than a passing acquaintance with either instrumentation and computers, or the intricacies of gas-phase ion chemistry. On the other hand, there are laboratories expert in reaction dynamics, collision processes, or geochronology who might be hard put to interpret the electron impact mass spectrum of an organic molecule.

After an interim decade or so of empirical spectrum/structure correlation studies, the analytical organic aspects are once again facing the problems of the real complexity in mixtures of substances which tend to characterize research problems from biomedicine to ecology, many times having to settle for the detection of one or a handful of components for the time being. However, new techniques such as chemical ionization, field ionization–field desorption, high resolution gas chromatography and high resolution mass spectrometry, and on-line minicomputers and microprocessors are providing a formidable, accurate and expedient arsenal for use in attacking these analytical problems.

In truth, the interests of mass spectrometry extend from mathematics, physics and chemistry through cosmochemistry and geology, atmospheric and environmental sciences to the biological and medical sciences, and beyond to such improbable disciplines as archaeology and history of art. The far-reaching effects of mass spectrometry are evidenced by imminent planetary studies within our solar system. This July, on the Viking spacecrafts, miniaturized Mattauch–Herzog double-focusing magnetic deflection instruments will be employed to measure the composition of the upper Martian atmosphere (*A5*), and soil pyrolysis Nier–Johnson type GC/MS instruments are then scheduled to land on Mars to probe the nature of possible carbon and volatilizable compounds on that body (*A1*). Such studies may leave a lasting imprint on theories concerning the origin of life and fundamental chemical evolution processes. Also, having developed high precision isotope ratio mass spectrometry, Wasserburg's group has just demonstrated an excess of $^{26}Mg$ in the Pueblito de Allende carbonaceous meteorite which is the first evidence for relatively large amounts of $^{26}Al$—now extinct—in the initial few million years during the formation of our solar system (*A3*). Such a heat source could have melted objects in the kilometer diameter category. In addition, high precision isotopic analysis of Pb has been carried out on as little as $8 \times 10^{11}$ Pb atom (*A8*).

Thus, if diversity and heterogeneity are conspicuous characteristics of mass spectrometry, then *clear, intelligent,* and *universally accepted nomenclature seems a necessity,* merely to retain an intact identity. Yet meaningful nomenclature is precisely what this subject lacks. What mass spectrometry does own is an enormity of jargon, local colloquialisms, confusing acronyms, and general balderdash. A step toward a remedy has already been made by the Committee organized by Meyerson et al. (*A4*), and the IUPAC Sub-Commission on Mass Spectroscopy established in 1973 is now considering the whole nomenclature question. Some early recommendations from IUPAC were contained in the report by Robertson (*A7*) and these are now being extended. The first set of recommendations of the Sub-Commission has been approved and will be published, first as "tentative recommendations" and then, eight months later, in final form according to the usual IUPAC procedure. Further recommendations will follow later.

One problem is that there are insidious advantages to maintaining a vague nomenclature. An impression of understanding can be given where none exists, and unjustified claims to originality can be insinuated when, in fact, the technique, mechanism, or whatever is derivative or a mere modification of previous well-established work. A case in point is the techniques all of which essentially measure the intensities of a particular ion mass or masses in the spectra of effluents from a gas chromatograph. The literature has been peppered with suggestions as to nomenclature without reaching consensus (*A2, A6, A9, D18*). Another example is the

A. L. Burlingame is currently research chemist and director of the Biomedical Mass Spectrometry Resource and related research programs at the Interdisciplinary Space Sciences Laboratory, University of California, Berkeley. He received his B.S from the University of Rhode Island and his Ph.D. from the Massachusetts Institute of Technology in 1962 with K. Biemann. He immediately joined the staffs of the Department of Chemistry and Space Sciences Laboratory and was assistant professor of Chemistry until 1968. He became associate research chemist in 1968 and research chemist in 1972. From 1964 to 1973, he was a member of several interdisciplinary scientific teams and committees entrusted with the planning and conduct of the lunar science program, and the preliminary examination and distribution of lunar samples from the U S. Apollo and U.S.S.R. Luna sample return missions During 1970–1972, he was awarded a J S. Guggenheim Memorial Fellowship which was spent on biochemical-biomedical applications of mass spectrometry with J. Sjövall at the Karolinska Institute, Stockholm. His research interests lie in the development of computerized double-focusing mass spectrometry, field ionization kinetics and Fourier transform $^{13}C,D$ nuclear magnetic resonance spectroscopy and their applications to biomedical and clinical research and organic ecochemistry.

Brenda J. Kimble received both her B.Sc. (Special Honors Chemistry) and her Ph.D. (Organic Chemistry, 1973) from the University of Bristol, England. Her thesis research utilized gas chromatographic and mass spectrometric techniques to study the organic geochemistry of triterpenoid hydrocarbons, and led to a publication which received the 1974 award from The Geochemical Society for the most outstanding paper published that year in the field of organic geochemistry. She joined the staff of the Space Sciences Laboratory, University of California, Berkeley, in 1973 and is presently assistant research chemist and assistant director of the Biomedical Mass Spectrometry Resource. Her research interests include the application of GC and MS for the determination of the molecular composition of complex biological and environmental mixtures, and in particular she has been involved in the development of capillary column GC/high resolution MS combination and in the design of appropriate computer techniques for data interpretation. She is a member of The Chemical Society, the American Chemical Society, and the American Society for Mass Spectrometry.

Peter J. Derrick has recently moved from University College London, to join the Department of Physical Chemistry at La Trobe University, Melbourne. He gained his B.Sc. (Special Honors Chemistry, 1966) and Ph.D. (Physical Chemistry, 1969) at King's College London, the latter under the supervision of A. J. B. Robertson. His doctoral thesis described a method in field ionization for determining ion lifetimes as short as picoseconds; this type of work has since come to be known as "field ionization kinetics". Awarded Fellowships by the Royal Society and the Royal Swedish Academy of Sciences, he spent some 14 months at the Royal Institute of Technology, Stockholm, studying aspects of molecular spectroscopy with Einar Lindholm. During 1971–1972 he worked in the Berkeley Mass Spectrometry Group, and directed the group during A. L. Burlingame's absence on Guggenheim leave. From 1973 to 1975, he held a Ramsay Memorial Fellowship at University College London, and lectured in physical chemistry. His research interests center on mass spectrometry, in particular field ionization and field desorption, and at the 1975 Gordon Conference on Analytical Chemistry, he was the Invited Discussion Leader for the mass spectrometry sessions. He remains deeply interested in both the practice and philosophy of teaching science, and he is an enthusiastic member of the Royal Institute of Chemistry, the Chemical Society, the Royal Australian Chemical Institute, and the American Society for Mass Spectrometry Dr. Derrick was the 1974 recipient of the Meldola Medal and Prize, awarded by the Royal Institute of Chemistry to the most outstanding young chemist of British nationality.

---

term "atmospheric pressure ionization" which could easily become misleading. There are already two types of experiment referred to by this term (*P10, P13*), and also a third ("plasma chromatography") which could be, but isn't (*P30–34*); "chemical ionization at atmospheric pressure" might be an adequate description for the Houston variation (*P5, P6, P9, P10, P19*). To distinguish chemical ionization with certain reagent gases from chemical ionization in general by speaking of "charge exchange mass spectrometry" (*P27*) can be confusing and does not really seem to be necessary. "Field desorption" and "field ionization" mean sample-handling techniques in organic mass spectrometry but are fundamental processes in physics and physical chemistry; to compound the problem, the ionization following the sample handling technique "field ionization" with an organic compound generally involves the "processes" of field desorption as well as field ionization. Another example concerns the terms "quasi-" and "pseudo-" with respect to "molecular ions" which are not observed as such. Quasi- and pseudo-molecular ions presumably yield quasi- and pseudo-molecular weights! "High resolution" is another problem. As an adjective it occurs as "high resolution GC/MS," or "GC/high resolution MS," or "HRGC/HRMS," while both the chromatographic and mass spectrometric resolution may have been practiced at any unspecified resolution. Also, the value of $M/\Delta M$ at which the resolution may be described as "high" is somewhat subjective.

The jargon effectively obviates reasonable peer reviewing and editing standards as the number of journals which accept papers dealing with mass spectrometry continues to proliferate.

Since the IUPAC committee has authority over the clarification of nomenclature which will be accepted by the journal population, it is hoped that, under Beynon's leadership, this terminological jungle will be cleared out in a nonpartisan fashion, resulting in nomenclature which will accurately reflect the expert practitioners' definitions of the phenomena in question.

## SCOPE OF THIS REVIEW

The work in mass spectrometry as reflected by the number of papers has increased again, and selection of subjects to be covered by this review is unavoidable. We adopt the same criteria for selection as previously (*B4*). Thus, after initial sections on instruments, techniques, and computers, we distinguish between developments in ion chemistry and analytical applications. We cover organic in preference to detailed treatments of organometallic, coordination and inorganic (*B39*) chemistry which are available (Spaulding in *B16*), and, in the applications section, we focus on biomedical and environmental studies. We believe our literature survey has been close to exhaustive for North American, European, Japanese, and Australasian journals, though the number of papers was a factor of ten too large for all to be included in the review. Our coverage extends from the cutoff point of the previous review up until December 1975, in the case of American journals, and October or November for most others.

The literature is covered in the *Mass Spectrometry Bulletin* published from Aldermaston, England, since 1966 (*B20*); as we have indicated previously, coverage is exhaustive but quite slow. The mass spectrometry bibliography prior to 1966 may be found in volumes by Waldron for 1938–1957 (*B36*), by Elliott for 1958–1960 (*B7*) and by Mead for 1961–62 (*B24*). There are three international journals devoted entirely to mass spectrometry: *Biomedical Mass Spectrometry* (*B3*), *International Journal of Mass Spectrometry and Ion Physics* (*B15*), and *Organic Mass Spectrometry* (*B27*). The last two appear monthly, and the first bimonthly. The Mass Spectroscopy Society of Japan publishes a journal entitled *Mass Spectroscopy* (*B21*), and *GC/MS News* has now completed its third volume (*B22*); both are in Japanese. A book on gas chromatography/mass spectrometry (*B34*) and another on practical mass spectrometry for medical sciences have appeared in the Japanese language and may possibly be translated in the future (*B32*). The 1974 edition of the "Registry of Mass Spectral Data" consists of four volumes and compiles reproductions of 18 806 authentic mass spectra (*B31*).

The Seventh International Conference on Mass Spectrometry will be held in Florence, Italy, in August 1976, and the proceedings will be published as usual; the proceedings of the Sixth International Conference have already appeared (1091 pages; *B38*). The proceedings of the Annual Conferences on Mass Spectrometry and Allied Topics held in the United

States, the 22nd of which was held in Philadelphia, Pa., in 1974, and the 23rd in Houston, Texas, in 1975, are only produced for delegates and members of the American Society for Mass Spectrometry and are not available commercially. National mass spectrometry meetings are held annually in the United Kingdom, West Germany, and Japan. The annual international symposia on biochemical and medical mass spectrometry were held in Milan in 1974 and Sardinia in 1975; the proceedings of the 1973 meeting, also in Milan, has now appeared (*B10*). The proceedings of the 1973 Rueil-Malmaison International Meeting on Organic Geochemistry—in the "Advances in Organic Geochemistry" series (*B33*)—contains a variety of papers on applications utilizing mass spectrometry; the 1975 meeting was held in September in Madrid and the proceedings will appear (*AB87*). The proceedings of the Mexico City Symposium on the Identification and Analysis of Organic Pollutants in Water contains the status of GC/MS applications to trace organic composition of drinking, natural, and waste waters (*B17*). The proceedings at the 1974 NATO Advanced Study Institute on Ion Molecule Interactions held in Biarritz, France, has been published, and the volume contains articles by many of the world's leading figures in this field (*B2*).

The volumes on mass spectrometry in the "International Review of Science Physical Chemistry" (previously MTP) series (*B18*) and the "Specialist Periodical Reports" series (*B16*) are necessary reading. The Maccoll Volume contains chapters on ion lifetimes (Derrick), physical inorganic aspects (Flesch and Svec), negative ions of organic, organometallic, and coordination compounds (Bowie and Williams), heavy-atom isotope effects (Shiner and Buddenbaum), ion kinetic energy spectroscopy (Beynon and Cooks), isotopic labeling for elucidating fragmentation mechanisms (Holmes), and quadrupole mass spectrometry (Todd and Lawson). The "Specialist Periodical Report" contains chapters on theory and energies (McMaster), structure and mechanism (Bentley), alternative methods of ionization (Wilson), computers (Mellon), organometallic and inorganic compounds (Spaulding), natural products (Games), reactions of positive and negative ions (Bowie), gas chromatography/mass spectrometry (Brooks and Middleditch), drug metabolism (Millard), and protein and carbohydrate sequence analysis (Morris and Dell). The first two chapters in the latter volume are fundamental and stimulating; however, both are misleading in parts (for example, on metastable studies and field ionization kinetics). In view of the general high quality and level of expertise assembled through what is now three volumes in this series, it is extremely unfortunate that these reports are not readily available to nonmembers of The Chemical Society, particularly in the United States.

Watson has written an introductory monograph oriented heavily toward biomedicine (*B37*). Using novel pedagogic format, it contains two chapters: one on qualitative applications, the other on quantitative applications, and 17 detailed appendices. The author states that the fundamentals can be read in a couple of hours.

Völlmin has written an introduction to biochemical mass spectrometry (*B35*), and the biomedical applications of selected ion monitoring have been exhaustively reviewed (*B9*; 135 references). The review volume on porphyrins and metalloporphyrins contains a chapter on mass spectrometry (*B30*). A recent review (396 references) of environmental applications of mass spectrometry is recommended particularly for its coverage of the compounds identified by this technique (*B1*). Chapman has prepared a book on computers in mass spectrometry (*B5*), and chapters on computer techniques for mass spectral library searching and cluster analysis (*B12*) and interpretation of mass spectra (*B29*) are available.

One of the volumes in the "Methods of Experimental Physics" series contains a chapter on mass spectrometry (*B23*), and there is a chapter on mechanistic aspects of mass spectrometry in Volume 1 of the "Isotopes in Organic Chemistry" series (*B14*). An overview of ion probe mass spectrometry has been presented (*B8*), and a book on methods of surface analysis contains chapters on secondary ion and field ion mass spectrometry (*B6*). A critical review of alloy thermodynamics by mass spectrometry has been published (*B28*) as well as one on the use of HRMS in the study of metallic systems (*B25*).

Two chapters by Green (181 references; *B11*) and Mandelbaum (*B19*) are in press on stereochemical aspects of mass spectrometry. Hesse has compiled the literature on indole alkaloids (*B13*), and "Progress in the Mass Spectrometry of Heterocyclic Compounds has appeared (134 references; *B26*), covering azoles, pyridine-carboxylic acids, polyazaindenes, 7- and 8-membered heterocyclic rings, chromene derivatives, and heterocyclic rings containing Group IV and V elements as hetero atoms.

Additional reviews of specific areas covered in the following sections include: modulated beam mass spectrometry (*C24*); modern ionization techniques (*P40*); GC/MS in pharmacology and toxicology (*D19*); computer-aided interpretation of mass spectra (*E5*); pattern recognition and learning machine approaches to interpretation (*E21*); mass spectrometry and computers (*E7*); EI decomposition processes of bifunctional molecules (*F5*); ring contraction processes (*F6*); the McLafferty rearrangement (*F28*); field ion kinetics (*G2, G3*); interpretation of appearance potentials (*H3*); unimolecular reactions (*K7*); molecular orbital calculations (*L30*) of carbocations (*L16*); mass spectrometry of negative ions (*M7, M8, M16*); field ionization MS (*N33*); field desorption MS of organic compounds (*N11, N12, N43, N44*); chemical ionization MS (*P30, P37, P40, P48, P51*); flowing afterglow techniques (*T2, T19*); MS and nucleic acid chemistry (*V7*); structure analysis of natural carbohydrates (*W14*); GC/MS of large polar lipids (*X37*); MS of prostaglandins (*Y2*); quantitative MS analysis of prostaglandins (*Y10*); mass spectra of biochemical compounds (*Z83*); MS and clinical chemistry (*Z18, Z30, Z44*); clinical applications of GC/MS (*Z29*); mass spectrometry of blood and respiration gases (*Z43*); MS in pesticide chemistry (*AB52*); GC/MS with EI and CI in the study of environmental health problems (*AB88*); sample handling and introduction techniques for GC/MS analyses (*AB20*).

## INNOVATIVE TECHNIQUES AND INSTRUMENTATION

Mass spectrometry has never been a field driven by commercially available instrumentation. Its lifeblood is created through the intimate interaction of the physical, instrumental, and computer scientists, with the organic and life scientists faced with the problems of probing and understanding the nature of living systems. As one forum for this expression and cross-fertilization, it is of interest "... to note that 23 years after the first mass spectrometry conference in Europe (held in Manchester in 1950) at least 26 of the 126 contributed papers were devoted to new instruments and techniques" (*C55*).

Meetings of the American Society for Mass Spectrometry (see section on scope of the review) have always emphasized the lure of new techniques and instruments and foreseen major thrusts into new fruitful applications. As these pioneering accounts become refined, they reach the scientific audience through publications in the original literature (see section on scope of the review). But a critical assessment of this aspect has not found its way, for example, into the "Specialist Periodical Reports" (*B16*).

Recently, in connection with the availability of a new modulated beam mass spectrometer, the basic features of this technique as well as its conjunctive use with phase spectrometry have been reviewed (*C24*). Such a combination of techniques can distinguish a radical from an excited molecule containing the radical. In addition, alternate means of detecting excited species are described, including ionization below the threshold of the ground state excitation, dissociative attachment to form negative ions, and associative ionization. Using phase spectrometry, it was shown that (for reasons unknown) when $SF_6$ was examined under high temperature conditions with a view toward determining the equilibrium constants for dissociation, it was not simply coming into dissociative thermal equilibrium with the furnace walls. This has raised the question of how fully equilibrated the Knudsen cell sources are in molecular beam type experiments which have provided much of the tabulated thermodynamic data. Studies of gas-phase oxygen radiolysis flow systems using modulated molecular beam mass spectrometry have led to a modification of the chemical model and the excited vibrational state of $O_2^*$ is postulated as a precursor to ozone (*C38*).

Improvements in quadrupole instrumentation developed for the study of neutrals have led to higher sensitivity, the ability to obtain the mass spectrum of neutral fragments, and determination of the appearance potentials and vertical ion-

ization potentials of neutral fragments (*C57*).

Fite's application of phase-angle spectrometry, in conjunction with other techniques, has made possible the study of low temperature combustion of acetaldehyde at sensitivities several orders of magnitude higher than previously (*C68*). Hence, the transient species methylhydroperoxide was observed in the flame profile. Additional studies of the acetaldehyde flame adding the fire-retardant $CF_3Br$ showed the presence of $CH_3Br$, $Br_2$, and HOBr. These methods should prove useful for the analysis of many dynamic systems, such as lasers, plasmas, flames, and atmospheric contaminants (*C67*). Pyrotechnic flames have been investigated by molecular beam time-of-flight mass spectrometry at atmospheric pressure (*C8*). Experiments on the HCN-laser plasma with a quadrupole have shown that molecular hydrogen is required as a collision partner for the 337-μm emission of the HCN laser (*C60*). The use of cylindrical Langmuir probes as a diagnostic technique for investigating drifting plasmas containing negative ions, such as $(O_2)^-$, $(NO_2)^-$, in the lower ionospheric region has been discussed. A plenary lecture on the techniques of mass spectrometric monitoring of ions in plasma emphasizes the theory of ion extraction through an orifice, the characteristics of biased monitoring orifices, ion optical effects, and design and performance requirements of the monitoring systems (*C31*).

Studies have been carried out on the adsorption of CO, $CO_2$ and $O_2$ in a closed system (*C35*). An equilibrium sorption study on ethanol, water, and polyurethane has evaluated the clustering functions in the polymer matrix (*C34*). Multichannel scaling up to 10 MHz was used to measure rare gas isotopic compositions at partial pressures below $10^{-15}$ Torr (*C49*). The realization that sodium and potassium, the sixth and seventh most abundant elements on Earth, are common impurities in almost everything (including dusts and smokes of virtually all kinds) and that these atoms are efficiently detected by surface ionization has been used to study airborne and other particulates and their size distributions (*C50, C51*). Such particulates strike a hot metal surface, melt, decompose, or pyrolyze and transfer their alkali impurities and surface ionize, yielding a burst of ions to be measured. In an attempt to introduce thermally unstable, low vapor pressure substances into a mass spectrometer ion source, atomization of a solution of such a substance is carried out resulting in aerosol formation. This aerosol is allowed to impinge on a plate directly above the electron beam of the ion source. Using EI/MS of these aerosols, dicarboxylic and higher acids, sugars and amino acids, ascorbic acid, and arginine were found to yield molecular ions (*C29*).

A technique, wholly new in concept, has been reported for the study of nonvolatile polar and thermally labile molecules (*C63*). The technique employs a $^{252}Cf$ fission source, the radiation from which strikes a 1-μm-thick nickel foil upon which a solid film of the sample has been deposited. The film is deposited on the far side of the foil from the source. The impact of the radiation upon the foil produces a thermal spike which vaporizes mobile impurity ions, which in turn ionize the sample. Mass measurement is by time-of-flight mass spectrometry using the radiation from the $^{252}Cf$ as time-zero. Typically the mass spectrum is dominated by an intense peak in the molecular mass region. Arginine and cystine have been studied (*C63*) and two tripeptides, Gly-Leu-Ala and Ala-Leu-Gly (*C40*). The tripeptides include the attachment of up to three sodium ions in the spectra. The spectra of neurotoxins such as tetratotoxin and atelopidtoxin have been reported (*C42*). The technique is a possible competitor for FDMS; however, it is difficult to evaluate from the limited information presently available. One factor to be considered is the potential danger in handling this radioactive material. Techniques for the storage of ions for up to 3.5 ms in quadrupole ion traps have been used to study chemical ionization processes (*C6, C15–C17, C48*). A rapid heating technique for substances on Teflon has been of advantage in peptide analysis (*U2, U3*).

Some interest has arisen in use of the matrix isolation technique to preserve ionic species for subsequent analysis by a GC/MS (*C13*). Comisarow and Marshall have explored the development of Fourier transform ion cyclotron resonance spectroscopic techniques. Mass spectra can be produced $10^4$ times faster than conventional ICR instruments or 100 times more sensitive, and operated at 10 000 resolution to produce automatically calibrated mass spectra. It appears that the high resolution capability observed at *m/e* 28 falls off dramatically with increase in mass (*C12*, and references therein).

A high resolution electron spectrometer has been attached to a scanning transmission electron microscope in order to determine the focusing properties of a spectrometer of this general kind in the energy range of interest in biological applications (*C37*). Ion implantation is becoming a major technique for the preparation of semiconductors and for purposes of understanding radiation damage of minerals and crystals (*C14, C18*), even for study of solar wind implantation into crystals on the surface of the moon (*C5*). Ionic analyzers and ion microprobes have been utilized to measure the depth profiles of particular species (*C4*). Ion microprobe analysis of the implantation depth profile has been reported with a resolution of 20 Å (*C43*). The value of high resolution mass analysis and concomitant exact mass measurement techniques has been illustrated in the characterization of secondary ion mass spectra from complex materials such as minerals, glasses, and ceramics (*C2*). Radiofrequency discharges in argon have been used to sputter and ionize solid samples for analysis of metals and substances deposited from solution (*C19*). This technique may be useful for studying the concentrations of minor elements in bulk metal samples.

Exploratory work using ruby-laser microprobe mass analysis of organic materials of interest in the cellular and subcellular transport of metal ions has been described (*C32*). Pyrolysis mass spectrometry of complex biological substances has been given some impetus using a carbon dioxide laser where higher reproducibility has been demonstrated even for bio-polymers, whole cells, and bacterial cultures (*C47*). Ruby-laser pyrolysis and GC/MS analysis of polymers has been used to assess the degree of deterioration of weathering of fiber glass–epoxy resin type composite systems (*C46*). Comparison of the laser-pyrolysis, GC/MS analysis of neutral lipids in both inert and oxidizing atmospheres has been presented (*C45*). Choline and acetylcholine in tissue samples have been analyzed by pyrolysis GC and GC/MS (*C62*). Pyrolysis GC/MS has been used to study the course of thermolytic reactions involving eliminations and ring closures, using the formation of isoindoles and benzofurazanes. Direct insertion of lyophilized gram negative bacteria into the ion source at 300 to 350 degrees produces mass spectra shown to result from pyrolysis products of phospholipids and ubiquinones (*C1*).

A detailed review containing 325 references of modern ionization techniques in mass spectrometry is recommended reading (*P40*). Field ionization and chemical ionization are emphasized. Design of a combined EI, CI, DI, and FD source has been detailed (*C27*) as well as a tandem EI/CI source (*C33*). Comparison of the FD, CI, and EI mass spectra of some steroids has appeared (*C30*). Peak matching has been applied to accurately measure the molecular masses of field desorbed ions for nonvolatile and thermally labile compounds, such as 6-mercaptoguanosine and 6-amino-hexanoic acid. A list of 18 useful FI/FD reference compounds is included (*C44*). A series of oligomers based on the $-CF_2-CF_2O-$ unit with aromatic end groups has been developed which shows promise for reference compounds for mass determination above mass 1000 (*C36*). Applying the previously reported electrohydrodynamic ionization source, solutions of sucrose or proline were added to glycerol as the host fluid with sodium iodide as the electrolyte. The mass spectra were predominantly composed of a series of glycerol polymers with sodium cation or proton attached and peaks in the spectrum characteristic of the added compound. Molecular fragmentation was minimal in these studies (*C61*).

Using benzhydryl ethers as test compounds, a claim to improved sensitivity on an MS 902 has been made by employing silanized quartz probe tips (*C56*). Hollow fibers, 150–200 μm o.d. with 25-μm wall thicknesses, were evaluated as sampling devices for trace volatile contaminants in aqueous solution and in air. Silicone rubber appeared most useful because of preferential permeability for volatile organics, pressure reduction, and enrichment of volatile organic compounds from aqueous solution and air (*C64*). Measurement errors due to depletion of blood gases in the vicinity of a diffusion membrane catheter coupled to a mass spectrometer have been compensated for by using an argon correction factor (*C54*). XAD-4 resin packed in borosilicate glass capillaries is proposed as a fraction collector for gas chromatography for batch

mass spectrometry (*C65*). A double collector magnetic instrument for the analysis of H, D, C, N, O, and S isotopes is aimed at the analysis of very small samples, 30 μg of carbonate and complete automation (*C7*). Ion counting and computer control have been incorporated into an isotope ratio mass spectrometer, yielding a precision of 0.5 per mil standard deviation and a minimum total sample size of $10^{-7}$ gram carbon as carbon dioxide (*C59*). A balloon-borne quadrupole has been constructed to measure the neutral and ionized constituents of the stratosphere in the 40-km region from mass 1 to 150 (*C53*). A multichannel mass spectrometer has been patented for analysis of breath atmospheres in submarines and space capsules (*C41*).

A low-noise detector for micro impurity analysis with a quad has been developed using off-axis techniques with an electrostatic deflector plate and a channel electron multiplier (*C52*). Ion currents in the order of $10^{-18}$ A can be detected. Microchannel electron multiplier arrays have been used in the focal plane of double-focusing Mattauch–Herzog ion optical instruments (*C3, C20, C28*). The channeltron with its fixed number of elements of finite dimensions may be the component limiting mass resolution in such a detection system. In the first paper, an ion current of 40 ions per second could be measured with a signal/noise ratio of 2 over a measurement time of less than a minute. Design curves have been presented for several analog and digital filters for use in filtering mass spectrometer data (*C9*). The design of an easily constructed sensitive molecular beam detector suitable for molecules which can be surface ionized ensures an ionization yield of 100% for such molecules (*C23*). Digitally controlled computer compatible quadrupole mass spectrometers (*C21*) and an electrostatic scanning GC/MS have been described (*C11*). An operating mode using a rectangular wave form and the requirement of keeping timing parameters steady may be used for high precision applications of quadrupole mass spectrometers (*C58*). Mass resolutions in the order of 3000 have been demonstrated using quadrupole mass filters (*C25*). The use of double-beam double-focusing mass spectrometry has been discussed for CI and FD applications. Accurate mass measurement of CI and FD spectra may be obtained using the EI-PFK beam (*C66*). It has been shown that metastable peaks can be measured under high resolution fast scanning conditions (*C10*). It has also been shown that simultaneous variation of the acceleration and electric sector voltages of a Nier–Johnson double-focusing mass spectrometer produces a spectrum of daughter ions derived from a selected metastable parent ion. The spectrum contains peaks which are not diffuse, such that precise mass measurement is facilitated in peaks due to isobaric daughter ions (*C39*). Variation of the resolving power of a mass spectrometer with variation of pressure within the analyzer tube has been studied using rare gas ions (*C26*). The design, performance, and versatility of an ultrahigh resolution mass spectrometer, the AEI MS 5074, has been described. Operation in excess of 10 000 and up to 150 000 may be obtained. Various schemes permit metastable scanning using different combinations of the instrument operating parameters (*C22*). Using the MS 5074, scanning at resolving power of 70 000 was illustrated using sulfur-containing petrochemicals. The $C_3$ vs. $SH_4$ doublet was resolved up to mass 240 (*C39A*).

## CHROMATOGRAPHIC–MASS SPECTROMETRIC–ON-LINE COMPUTER TECHNIQUES

Once again Brooks and Middleditch have prepared a comprehensive treatment reviewing all aspects of the new advances in methodology and extensive applications of GC/MS through June 1974 (592 references, *D7*). It is mandatory reading for its breadth of analytical applications to bioorganic chemistry, medicine, food chemistry, geochemistry, and environmental chemistry. A report on the state of the GC/MS art in pharmacology and toxicology, including the role of stable isotopes for quantitation, contains 70 references (*D19*). A fruitful and rewarding level of excitement obtains in this field as the marriages between the differing components of a stand-alone system become optimized, including chromatographic resolution, mass resolution, and mass spectrum scan cycle time. Mass spectral sensitivity and mass resolution with concomitant high accuracy of mass measurement permitting assignment of elemental compositions are being developed and explored. Routine high performance and reliability are becoming established using support-coated open tubular (SCOT) glass capillary gas chromatographic columns and wall-coated open tubular (WCOT) glass capillary columns and require special techniques for the versatile physical coupling of such glass capillaries to the ion sources of mass spectrometers.

Three types of connection techniques are still being developed and evaluated with respect to overall system chromatographic resolution, performance, and sensitivity. These are the direct connection, open-split connection, and the separator (*D29*). A suitable direct coupling using an all-glass interface containing a restriction was designed for an AEI MS-12 spectrometer. Good spectra were obtained from less than 10 ng per compound injected on the GC column (48-m, 0.25-mm i.d. OV-101) and showed no deterioration in total ion current profile compared with flame ionization detection profile; however, the reconstructed total ion current profile was not shown. The open-split connection of a glass capillary column using a platinum capillary inlet line to the ion source permits operation of the exit of the column at atmospheric pressure and facilitates intercomparison of capillary performance and retention indices with a flame ionization detector (*D51*) as well as the mass spectrometer. This device permits operation at up to 100 000 effective plates with no peak broadening or tailing caused by the interface (*D29*). For CIMS, the reactant gas is added through a glass tube placed coaxially around the Pt capillary (*Z21*). Using the open-split type connection also permits dilution of chromatographic peaks that have too high a concentration as well as trapping of broad peaks, i.e., toward the end of a GC run, with subsequent rapid evaporation to increase the maximum concentration in the ion source. On-line hydrogenation can also be carried out. The main advantages of the open-split connection are 1) atmospheric pressure at the end of the column, 2) maintenance of chromatographic resolution, 3) versatility with respect to column types and flow rates, 4) rapid and safe changing of columns, and 5) very high reliability.

A quadrupole mass spectrometer has been utilized inside of a magnetic instrument as a total ion current detector (*D30*). A comparison of the signal-to-noise characteristics of WCOT, SCOT, and packed columns has been presented and a case made for the use of the double-stage Becker–Ryhage separator to maintain ion source focusing characteristics with a standard vacuum system and increase overall GC/MS sensitivity. Less than 25-ms exposure time to the stainless steel double jet is suggested as a reason for the chemical inertness of this separator-type GC/MS system (*D17*). Using glass micropack columns, very polar compounds have been run on a directly coupled GC/MS arrangement with no loss in chromatographic resolution (*D8*). Chromatograms of aliphatic alcohols, low boiling free acids, and low boiling free amines were presented as examples. A flexible sample transfer line from any gas chromatographic FID tip to a quadrupole mass spectrometer has been described (*D22*). Using an effluent splitter with delay line and effluent recombination such that the delay corresponds to the peak width at half height yields square top GC peaks. This peak squaring technique may have advantages in recording mass spectra from chromatographic columns (*D61*).

An all-glass remotely controlled high temperature valve for venting in a GC/MS interface has been described (*D39*). Also, a diverter valve for GC/MS has been described which permits venting of the solvent front or undesirable peaks in the chromatogram (*D63*). A fast scanning GC/MS magnetic sector instrument has been described employing capillary columns and scan speeds of 0.7 s for the mass range 5 to 500 with a cycle time of 1.4 s (*D26*). The value of high resolution glass capillary column mass chromatography in combination with combined EI and CI quadrupole mass spectrometry has been demonstrated with 1-s scan times. Polynuclear aromatics, a sample of oil, and a mixture of sterol methyl ethers were employed to show the relative advantages of the CI and EI modes of its operation (*D21*). Exchange of labile hydrogens for deuterium has been demonstrated for capillary GC CIMS (*D55*).

While GC/low resolution mass spectrometry (LRMS) is commonplace and high resolution GC/LRMS is developing rapidly, the optimization of chromatographic resolution and mass resolution with concomitant formidable data management problems including the acquisition and processing of accurate mass and elemental composition information has only begun. A review of the development of packed column

GC with high resolution mass spectrometry (HRMS) has been presented in connection with the development of routine packed column GC/real-time HRMS (*D35*). A 10-foot, 1/16-inch i.d. stainless steel packed column coated with Dexsil and connected via a single-stage stainless steel jet separator to an AEI MS-902 was used on-line to a preliminary version of the LOGOS II–Sigma 7 real-time computer system; an evaluation of mass measurement accuracy was carried out using scan rate of 8 s per decade and a dynamic resolution of 10 000 (*D36*). The scan cycle time was 23 s from mass 800 to mass 20. Digitization rates of 50 and 100 kHz were compared with respect to mass measurement accuracy and showed 98% of the mass measurements within 10 ppm and 75% within 4 ppm. The recording of continuous high resolution mass spectra throughout a GC/HRMS analysis of permethylated pooled normal urine yielded the first examples of the usefulness of the new technique, elemental composition chromatography (accurate mass chromatography).

The use of gas chromatography with high resolution mass spectrography of Erythrina alkaloids was discussed using resolution of 20 000 and photoplate recording using Ionomet photoplates. It was stated that this technique can give accurate mass measurements for components in the order of 50 ng on 30 to 40 peaks in the mass range 100 to 500 (*D25*). Further work with the AEI MS-3074 double-beam, double-focusing mass spectrometer has demonstrated 1 s per decade scans with the production of accurate mass measurements of EI, CI, and FD spectra (*D3*). Using PFK as an internal standard and resolution sufficient to resolve certain organics at $m/\Delta m$ 3000, certain exact masses have been obtained for compounds up to molecular weight 215 with 3 s per decade scan times using a Varian MAT 311a mass spectrometer and a glass capillary (*D54*). The dynamic ranges reported vary from 18 to 48 in the mass calculations presented; in general, peaks below mass 70 were not reported. Burlingame and co-workers have further developed real-time HRGC/HRMS to permit operation with glass SCOT capillary columns for the analysis of complex mixtures of organic substances (*D37*). The scan cycle time has been dramatically decreased to 9.6 s covering the mass range 800 to 60. Experiments were carried out to evaluate mass measurement accuracy using the 9.6-s cycle time at 10 000 resolution operating with the SCOT capillary column inlet. Fifteen selected nitrogen-containing ions covering the mass range 114 to 614 were utilized to evaluate the mass measurement accuracy. One hundred percent of the mass measurements were less than 17.5 ppm and 96% were within 10 ppm. The dynamic range was greater than 130 to 1. Using the SCOT column, methyl stearate eluted in about 20 s and, hence, approximately two high resolution mass spectra were obtained per peak elution profile. The operational version of LOGOS II permits the recording and real-time display of *any number of high resolution mass spectra*. Typically, 300 to 400 high resolution mass spectra are obtained from an open tubular capillary column run. Using this technique, the analytical advantages and specificity of elemental composition chromatography (ECC) have been demonstrated for the studies of composition of physiological fluids, as well as municipal and industrial wastewaters (*AB18, AB19*).

A recent editorial concerning present problems confronting analytical chemists faced with the analysis of complex mixtures containing hundreds of components, such as physiological fluid analysis and environmental samples, correctly realized that current instrumental techniques can be developed and employed to either characterize hundreds of components in a mixture or very specific components in mixtures containing thousands of components (*D40*). However, it is premature to have drawn the conclusion that HRMS techniques are being misused when applied to such difficult problems facing analytical chemistry. It seems ill-timed to make such an assessment when development of HRGC, HRMS, and computer management of these spectra is proceeding at such an exciting pace. Decafluorotriphenylphosphene has been proposed as a reference compound to evaluate GC/MS systems including their on-line data systems (*D14*). It, like many other compounds, is of reasonably low molecular weight. It would seem that something of twice that molecular weight, ~800–1000, might be more appropriate.

Selected ion monitoring (SIM), initially called mass fragmentography, also goes under the guise of multiple ion detection, selective ion detection, ion specific detection, multiple ion monitoring, multiple mass monitoring, multiple ion analysis, tuned ion analysis, selected ion peak recording, and others (*D18*). The earlier authoritative review of SIM in neurobiology is recommended reading since it also contains an exhaustive bibliography up to 1973 (*D11*). The bibliography has now been supplemented to cover the literature to the beginning of 1975 (*D52*). An exhaustive review of the biomedical applications of SIM has just appeared (*D18*). Discussion includes magnetic sector instruments, quadrupoles, time-of-flight, modes of operation of the instruments, instrument operational parameters, computers, and quantitative SIM. The final section is on applications of SIM to a host of biomedical problems. Computerization of this technique for the LKB 9000 GC/MS using a minicomputer and adjustment of the accelerating voltage for a maximum of 8 masses within 30% mass range has been described in some detail (*D24*). A similar description has appeared for applications using a quadrupole mass spectrometer (*D20*). An instrumental development extending the range of applicability of this technique for several components in a GC run has employed both the computer control of the accelerating voltage and the magnetic field. The maximum time required for a magnetic field change is 8 s, whereas of course the accelerating voltage changes can be carried out in milliseconds (*D64*). The fundamental limitations in the precision of this method of measurement of isotope ratios from GC/MS have been discussed in terms of the number of measurement cycles and the effects of the pattern of observation used in the Gaussian-shaped GC peaks (*D43*).

A comparison of integrative recording techniques for SIM has been carried out (*D42*). A computer-controlled continuously rescanning subset data acquisition technique was applied to the analysis of polychlorinated biphenyls from environmental samples (*D15*). A stable isotope ratiometer, SIM unit has been designed and constructed which can drive a GC quadrupole or magnetic sector instrument to monitor up to six ions in turn (*D38*). This has been illustrated by analysis of mono-, di-, and tri-hydroxy bile acids. A comparison has been made of the unlabeled and labeled internal standards for quantification of methylated alobarbitone using a GC quad (*D41*). A focus and threshold monitor has been described (*D53*). An interface for a quadrupole to a laboratory minicomputer for automated SIM has been described (*D59*).

Liquid chromatography (LC) continues to develop rapidly, especially for the separation of compounds that are higher molecular weight, and thermally and chemically labile. Hence, the interest in utilization of mass principles for detection of liquid chromatographic effluents continues. The problem, of course, is the interface. A silicone rubber membrane molecular separator has been employed which permits the transport of nonpolar molecules for mass spectrometric characterization (*D33*). A second interface type consists of differentially pumped chambers and a wire train which continuously takes samples from the LC effluent, evaporates the solvent and vaporizes the solute in the ionizing chamber of the mass spectrometer (*D58*). The third takes 1% of the LC effluent for introduction directly into the ion source of the CI mass spectrometer. In this case, the solvent acts as the ionizing reagent at relatively high source pressures. McLafferty and co-workers have explored this technique to some considerable extent and are looking toward promising applications in the characterization of small oligopeptides (*D1, D2, D45, D46*).

The availability of minicomputers with suitable disc-oriented operating systems, graphic display units, and electrostatic printer plotter units as well as the continually increasing performance/cost ratios are in the process of completely revolutionizing and facilitating the techniques of mass spectrometry. This is particularly true for GC/MS where the continuous repetitive scanning of mass spectra can be recorded, manipulated, monitored, and interrogated in essentially real-time. More and more, highly detailed information is obtained on the composition of extremely complex mixtures of organic substances as the resolution of gas chromatography advances with the advent and application of open tubular glass capillaries.

Computerized data acquisition, processing, and management of mass spectra have become a crucial and extensive field which is in the early stages of exploratory networking. An excellent updated review by Mellon of computerized data acquisition and interpretation has already appeared (*D48*).

A monograph by Chapman is in press (*B5*). Hence, only the salient developments will be mentioned here.

Utilization of a microcomputer as a high speed oscillograph for GC/MS illustrates its use as a buffer memory (*D23*). Microprocessors will certainly once again dramatically enhance the performance/cost ratio for the management of mass spectrometer functions via computer techniques. A mass marker technique has been described for mass calibration in a data system based on a PDP-11/20 computer (*D27*). Several more sophisticated on-line computer hardware and software systems have been adapted for generalized utilization of on-line mass spectrometers under low and high resolution operations as well as GC repetitive scanning conditions. One system is a Ferrante Argus 500, 24-bit computer with 16K core (*D62*); another is a PDP-10, 36-bit computer with 96K core (*D28*); the third is a Xerox Sigma 7 with 32-bit, 96K core (*D9, D47*). While the goals and laboratory MS applications for these three types of on-line computer systems differ, they represent important advanced models for the future development of computer management of mass spectral data both in the on-line real-time "paperless interrogation" mode as well as the spectral archiving, file management, and networking modes.

A general method for molecular ion prediction using either low resolution mass spectral data or elemental compositions from accurate mass measurements has been presented (*D13*). Various uses of repetitively computer-acquired mass spectra have been discussed (*D31*). A specialized algorithm for the combination of mass chromatograms has been used for the detection of chlorinated derivatives of polycyclic aromatic hydrocarbons (*D10*). Principal component analysis or factor analysis is actively being explored as a means of establishing the multiplicity of components in a single chromatographic peak from GC/MS data (*D12*). A more detailed discussion of data selection, and transformation, and factor compression and transformation has been presented in this connection (*D57*) using 22 isomers of alkyl benzenes with the formula $C_{10}H_{14}$ as examples (see also *E26*). Attempts have been made to relate functional group to mass positions using this technique (*D34*).

The correlation of simultaneously maximizing coeluting masses in repetitively scanned GC/MS data has led to a description of so-called reconstructed mass spectra (*D6*) which has proved to be an important clean-up step prior to the use of any file searching technique for computer identification of a high quality unknown spectrum. The inclusion of gas chromatographic retention indices in GC/MS data sets has been described for applications to biological mixtures by both Biemann's and Sweeley's groups (*D50, D60*). Data and coding techniques and procedures for component identification by reference to precoded data files have been described in connection with analysis of volatile components of foods (*D49*). Computer evaluation of GC/MS analyses has been applied to characterization of unlabeled and polydeuterium labeled compounds containing between 0 and 19 deuterium atoms (*D4*). The use of a computer-searchable collection of 300 mass spectra of drugs, metabolites, and normal body fluid constituents as well as contaminants has been described and its results from two years' use on some 600 patients presented (*AA21*). Speed, component, or mixture identification and specificity are key virtues of this approach.

A method has been described for extracting the chemical information from empirical formulas derived from accurate mass measurement by checking the self-consistency of the isotopic clusters (*D32*). A subroutine has been written to calculate elemental compositions from low resolution isotopic clusters. Of course, the ion–molecule reaction problem at higher source pressures and with polar materials will limit the usefulness of this technique as it has in the past (*D16*). Three complementary methods to determine accurate fractional abundances of isotopes from mass spectral data have been described (*D56*). FORTRAN IV programs capable of calculating all the possible mass values for up to six specific masses are available (*D5, D44*).

## MASS SPECTRAL MANAGEMENT AND INTERPRETATION TECHNIQUES

Mellon has brought the literature up to date as of June 1974, including library searching, heuristic and pattern recognition techniques for the interpretation of mass spectra (*D48*). The new "Registry of Mass Spectral Data" contains mass spectra of 18 806 different compounds (*B31*). The empirical occurrences of mass and abundance values in known recorded mass spectra have been characterized to mass 400 and have been used as the basis of attaching probability of occurrence as a function of mass window in McLafferty's probability based matching approach (*E30A*) (see below). Significant developments of mass spectral search systems are under way and will be particularly useful for routine identification of components whose spectra are in the files, providing that the unknown spectra are of sufficiently clean quality to ensure a highly probable matching factor. Techniques based on various criteria of selection of the peaks in a mass spectrum still continue to appear, such as using only the six most intense peaks of each library entry (*E35*). Compression techniques for data files have been discussed to reduce the required storage and speed the search of a library (*E33*). Grotch continues to develop his software incorporating an algorithm used to measure the "goodness of fit" in binary encoded mass spectra (*E15, E15A*). A combination of ion series techniques proposed previously by Smith, Gray, and Morrison, and "the profile of an unknown mass spectrum" have been described by Gray (*E10*). Other suggestions as to the computer classification of spectra with regard to their membership in groups of compounds have been articulated (*E9*). Identification of 5- and 6-membered naphthenes in mixtures has been described (*E3*). The literature is growing on McLafferty's self-training, interpretative, and retrieval system for mass spectra (STIRS) (*E30, E37*), including his probability-based matching (PBM) of mass spectra (*E29, E31*). The capability of STIRS has been extended to permit the compound selected as providing the best match to the unknown mass spectrum to be examined by the computer for the presence of each of 179 common substructural fragments (*E6*). The matching and interpretative aspects of these systems are now available over an international computer network from Cornell University through TYMNET (*E28*). The main problem with commercial and university computer centers and networking presently is the high cost per search or match or interpretation which is in the order of $2.00–10.00. The availability of the file spectra of most closely "fitting" candidates is a continuing frustration. These factors virtually preclude the routine usefulness in the sense of file search identification of continuously recorded mass spectra from gas chromatographic effluents from high resolution capillary columns. Reverse searching has been shown to be superior for identification of file components present in the mass spectrum of a mixture (*E2*). Another experimental international conversational mass spectral search system has been described (*B12, E17–E19*). Clerc and Erni have written a review on the identification of organic compounds by computer-aided interpretation of spectra, including algorithmic methods and comparison methods (*E5*). Programs for generating empirical spectrum classification schemes have been described (*E11, E13*) and utilized in screening GC/MS data on a laboratory computer (*E12, E14*). A program was developed for the interpretation of mass spectra of heterocyclic selenium and germanium compounds (*E23*). A plenary lecture on information theory in mass spectrometry emphasizes that the applications to date have been few and usually consist of well-behaved mixtures of known compounds (*E20*). Digital learning networks have been suggested as a solution to the automatic routine identification of mass spectral data according to the functional groups of the molecule present (*E36*). It is an embodiment of the *n*-tuple method of pattern recognition. A review of the pattern recognition and learning machine approaches to interpretation of mass spectra has appeared (*E21*). Another review of mass spectra and computers has appeared by Delfino and Buchs (*E7*). It has reviewed the learning machine, deduction programming, heuristic programming approaches. The application of learning machine techniques to the interpretation of mass spectra of monofunctional substances has been described (*E22*). A program using adaptive binary pattern classifiers has been developed to generate chemical structures from low resolution mass spectra (*E1, E39*). A method for the development of near-optimum linear discriminant functions for nonseparable analysis of mass spectra has been described (*E32*). These techniques have been used to interpret spectra of alkylthiol esters (*E16*) and *n*-acetylhexosamines (*E38*). A simplified learning machine has been used for the preliminary

classification of mass spectral patterns (*E25*). Performance of different methods of computer matching of mass spectra has been examined using a library of terpene mass spectra (*E27*). This has also been used for the identification of alkylbenzenes (*E26*). Further work on the applications of artificial intelligence for chemical inference in mass spectrometry has appeared (*E8*). An algorithm for finding complete sets of nonequivalent labelings of a symmetric object (*E24*) has been achieved. Such a technique has been used for the labeling of the polychlorobiphenyl hydrocarbons (*E34*), and a program called CONGEN provides the capability for ensuring that no plausible alternative structures have been overlooked in assessing the interpretation of a mass spectrum in terms of its fragmentation pattern (*E4*).

## TECHNIQUES IN ION CHEMISTRY

We build on the foundation laid in the previous review (*B4*), where most sections were prefaced by a few sentences of basic explanation about the technique. Ion–molecule reactions are again classified according to technique, although distinctions are sometimes rather fine.

**Electron Impact (EI) and Organic Mass Spectrometry.** Interpretation of electron impact (EI) mass spectra requires elucidation of the nature of gas-phase (radical-)ion processes and, particularly, their dependence on internal energy and molecular structure and stereochemistry. This knowledge is derived from specific labeling with stable isotopes (*B14, F12, F27, F33*), accurate mass measurements (*F3*), metastable measurements (*F35*) (see separate section on "metastables") and perhaps EI at low electron energies (<12 eV), and is formulated as mechanisms, the shorthand of chemical reactivity. The number of papers falling within this category is extremely high, so we select salient high-quality work for our coverage. There has been a review of decomposition processes of bifunctional molecules (*F5*), and a brief review of ring contraction (*F6*). The McLafferty rearrangement has been reviewed (*F28*).

One of the most active groups in these areas has been that of Nibbering et al. (*F10, F21, F45, F54, F57*), and we note in particular their studies of skeletal rearrangement of cycloheptatriene (*F56*) and sequential hydrogen shifts in the methyl ester of γ-nitrobutyric acid (*F40*). Together with Cooks, they have unearthed an example of two reaction channels leading from the same reactant $(CH_3CHO\text{-}CH_2OCH_3)^+$ to the same products $(CH_3COCHCH_3)^+$ and HCHO (*F46*). Djerassi et al. (*F4, F13, F24, F52*) continue to report steroid (lanostane, methylcholestane) studies of high quality (*F41*). Meyerson and Karabatsos (*F38*) have concluded that the loss of HCN from ionized propionitrile involves a 1,1-elimination, whereas H loss involves C-3 (see also *F39*). Pursuing their interests in concerted eliminations, Mandelbaum et al. (*F59*) have shown that certain *trans*-1,2-disubstituted cyclobut-3-enes decompose to a greater extent than their cis isomers. There has been a deluge of papers from Schwarz et al. (for example, *F29, F47, O27*), and the Norwegian series on onium compounds still seems vigorous at Part XXIX (*F18*). Rebane's series (for example *F42–44*) on organoselenium compounds could become the definitive work on this subject. A notably thorough example of a traditional EI study is that concerning the structure and ion decomposition of mevalonolactone (*F14*).

It has been proposed that, following EI of cyclohexanol at 70 eV, *highly excited* molecular ions delay for microseconds before fragmenting (due to the intervention of a long-lived acyclic isomer), although less excited molecular ions fragment in much shorter times (*G9*).

Stereoselectivity in EI-induced decomposition has been reported in several excellent papers (*F9, F34*), and stereochemistry in mass spectrometry has been the subject of two reviews (*B19, F15*). Stereospecificity in an ion decomposition provides some of the strongest evidence for reactant ion structure (*F15, G9*). There has been an ingenious investigation of the effects of transition state geometry in the McLafferty rearrangement (*F20*). It has been suggested (*F7*) that the processes responsible for isotopic hydrogen randomization in 2-methylpropane ions occur at high internal energies [unlike hydrogen rearrangements leading to isotopic randomization in unsaturated ions, which are favored by low energies (*G3*)] General long range interactions in large chains have been treated mathematically by a flexible chain model (*F61*). De Jongh et al. (*F31, F32, F50*) study analogies between pyrolysis and mass spectrometry (see also *F60*), and the general subject of thermolytic and photolytic comparisons in mass spectrometry has been reviewed by Dougherty (*F8*). Tsuchiya and Adachi (*F53*) have reported "excess kinetic energy spectra" produced by adjusting the repeller potential to suppress all ions but those with excess kinetic energies. Since the excess energy ions are generally formed only by direct cleavages, these spectra are not complicated by rearrangement ions and are more readily interpreted in terms of the structure of the neutral. A peak at $(M + 2)^+$ in the EI mass spectrum of polyporic acid is described as anomalous, and moves to $(M + 4)^+$ on introducing $D_2O$ into the source (*F16*).

We can merely reference some other papers loosely classified as being concerned with molecular radical-ion isomerization (*F1, F11, F19, F36, F51*), skeletal rearrangements possibly as an integral part of decomposition (*F2, F25, F26*), neighboring group participation (*F22*), temperature effects (*F23*), kinetic isotope effects (*F37*), stilbenes (*F17*), $(C_7H_7)^+$ (*F48, F49*), loss of HX from 2-haloethanol ions (1,2 elimination) (*F55*) and imines (*F30, F58*).

**Field Ionization Kinetics (FIK).** Field ionization kinetics (FIK) has been recently and comprehensively reviewed by Derrick (*G2*). From the point of view of elucidating the nature of gas-phase ion decomposition processes and the formulation of mechanistic rationale in terms of molecular structure and stereochemistry, perhaps the most important feature of FIK is that at the very short times (picoseconds) at which ion decomposition can be observed, the structure of a reactive molecular ion is likely to resemble that of its neutral precursor. Thus, it may be possible to delineate reaction pathways of known ion structures (*G18*). This assumption is implicit in the interpretation of FIK measurements on specifically deuterated alkenes (*G4, G5*), ketones (*G8*), and benzoic acid and toluene (*G14*). It is these and other measurements on isotopically labeled molecules which have led to the conclusion that "hydrogen randomization" in alkenes and ketones is the result of series of highly specific hydrogen rearrangements (accompanied by skeletal rearrangements in some cases) (*G3*).

The lifetimes and rates of decomposition determined by the technique are reproducible from laboratory to laboratory despite differing instrumentation and experimental techniques and differing methods of calculating the lifetimes, thereby engendering confidence in the accuracy of the data (*G10*; see also *G16*). Varying the energy resolution under which FIK measurements are made has shown that the widely used normalization procedure is generally reliable and does not introduce error into the *normalized rates* $k(t)$ (also referred to as phenomenological or average rate constants) (*G1*). There is still little detailed information concerning the excitation energy of the reactive molecular ions (*N19, N24*), although it has been suggested that there can be differences between stereoisomers in this respect (*G13*) and that energy deposition can be affected by "conditioning" of an emitter (*G10*). The kinetic data provided by FIK accord with the quasi-equilibrium theory inasmuch as for certain types of ion decompositions there are continuous distributions of lifetimes over 7 orders of magnitude of time and the dependences on time of the relative rates of parallel reactions show the qualitative trends predicted by the theory (*G3, G7, G15*).

Results on branched aliphatic aldehydes suggest that the McLafferty rearrangement proceeds through an intermediate and involves in some cases (at least) two distinct hydrogen transfer steps (*G6, G17*). Work on specifically deuterated cyclohexanols has revealed a previously unidentified 1,2 elimination of water (*G9*). Results for $^{13}C$ and $^2H$ specifically labeled methylcyclopentane suggest the existence of (at least) two pathways for both the loss of methyl and the loss of methane, one in each case from a ring-intact ion and the other(s) from ring-cleaved ions (*G11*).

Long ion lifetimes ($10^{-6}$–$10^{-3}$ s) following EI have been measured using the recently constructed tandem ICR instrument (*G19*). Dissociative lifetimes ($\sim 10^{-6}$ s) of $(CO)^{2+}$ have been determined in a time-of-flight instrument (*G12*).

**Appearance Potentials (AP's).** The most reliable methods of determining appearance potentials (AP's) employ photoionization (PI) or *energy-resolved* electron beams, and are capable of accuracies of better than 10 kJ $mol^{-1}$ for many

fragment ions and 1 kJ $mol^{-1}$ for molecular ions [ionization potentials (IP's)]. That the results from both methods are accurate, and not merely precise, is suggested by the generally good agreement between them. For example, electron impact (EI) and PI AP's for $(C_3H_5)^+$ from propene differ by no more than 6 kJ $mol^{-1}$ (*H5*). Where accurate EI and PI values do differ, it probably indicates the existence of internal energy states accessible through one but not the other ionization process. For example, that the PI AP of $(CH_2Cl)^+$ from $CH_3Cl$ was found to be an eV higher than the EI value has been interpreted as evidence of decomposition of an ion state accessible by EI but not by PI (*H1, H34*). Accurate AP's have been reported for formic and acetic acid (*H19*) (accuracy of ±0.2 kJ $mol^{-1}$ using PI for the ionization potentials), ethylene (*H26*) and a variety of small molecules (for example, *H6, H8, H27*). The angular distributions of dissociation products (which are anisotropic) from $H_2$, $N_2$, and CO have been measured using EI (*H21*). Double ionization of rare gases has been investigated using EI (*H17*). Photoelectron spectra have been reported for organic radicals (methyl, *tert*-butyl) (*H20*).

To obtain accurate AP's using electron beams with broad energy distributions, it is probably necessary to deconvolute the ionization efficiency curves. One successful approach (*H9*) using time-averaging to improve signal/noise ratios and Fourier transform deconvolution can now be carried out by means of an interactive computer program, which is available on request from Morrison. The single energy-distribution-difference (EDD) method of refining ionization efficiency curves has been employed and critically discussed by Gross et al. (*H13*) and by Johnstone and McMaster (*H18*). Occolowitz et al. (*H28*) have evaluated six of the more common methods of fixing onsets (see also *H10*). Some suggested improvements to the retarding-potential-difference (RPD) technique have been put forward (*H16, H30*).

One potential pitfall to the interpretation of AP's, a subject which has recently been discussed rather fully (*H3*), is the "kinetic shift" which represents an amount of energy in excess of threshold necessary for the ion to react sufficiently fast to be detected, given the ion-optical configuration employed. A successful approach to minimizing kinetic shifts has been to determine AP's of fragments from long-lived ions (in some cases $10^{-3}$ s), using ion trapping in the space charge of an electron beam (*H11, H23*) or ion cyclotron resonance (*H4*). The kinetic shifts observed with, for example, benzene or benzonitrile are large [up to 200 kJ $mol^{-1}$ (2 eV)]. On the other hand, kinetic shifts for many other ion decompositions are negligible, and accurate AP's are finding increasing use for the elucidation of ion structure [see for example the discussion by Holmes (*H15*) of the structures of $(C_4H_5)^+$, $(C_5H_7)^+$, and $C_5H_8)^+$]. The AP of a decomposition places an upper limit on the heat (strictly speaking, energy) of formation of the product ion, which may be sufficient information to identify its structure or at least exclude some possibilities (*H7, H22, H25, H31*).

The trend of the AP's for the loss of H· from cyclopentane, -ene, and -adiene clearly shows the antiaromaticity and consequent destabilization of the cyclopentadienyl cation (*H24*); Lossing continues to make some of the most accurate AP measurements on timely moieties. A point of interest from the EI study of deuterated ethylenes is that the AP's of $(CH_2)^+$ and $(CD_2)^+$ from $CH_2{=}CD_2$ are less than that of $(CHD)^+$ (18.7 vs. 20 eV) (*H32, H33*). Values reported by two different groups for AP's for loss of water from deuterated cyclohexanols disagree significantly (*G9, H12*). Some interest remains in substituents effects on AP's (*H2, H14, H29*).

**Translational Energy Release and Metastables.** During unimolecular decomposition, a proportion of the internal energy of the reactant is converted to translational (kinetic) energy of the products and, for a metastable process, this amount of energy can be determined precisely using a commercial mass spectrometer. For the purposes of this review, we define "metastable" as ion decomposition after a lifetime of microseconds (give or take an order of magnitude) (see *I32*). The metastable peak *shape* is measured under defined ion-optical conditions, and this reflects the translational energy distribution of the product ion which can be transformed by mathematical procedures to the *distribution* of internal energy converted to translation during decomposition (*I42, I43*; see also *I30*). The precision with which the energy released can be determined by this method arises because the reactant ion is travelling at high velocity (order of keV) and, hence, a *small* energy release during decomposition is seen as a *broad* translational energy distribution in the product ion (the characteristic broadness of metastable peaks) (*I42*; see also *I41* on the subject of precision).

The resurgence of interest in determining translational energy releases during metastable decomposition (*G18, I6, I46, I47*) is due in no small part to Beynon, Cooks, and colleagues, who have emphasized the significance of the measurements to understanding reaction processes and to energy partitioning (*I4, I8, I11, I23, I40*). Of particular note is the small energy release (17–45 kJ $mol^{-1}$) in the formation of $(C_6H_5CO)^+$ from α-halogenated acetophenones which is attributed to predissociation (*I7*), and the differing energy releases of 1,2- and 1,3-eliminations of HCl from chloroalkane and chloroalkene ions (*I25*). The large energy releases (several hundred kJ $mol^{-1}$) in the decomposition of doubly-charged tri-atomics can be rationalized in terms of transitions which conserve total spin and angular momentum (*I9*). The energy released in the metastable loss of H· from methane has been found to be dependent upon temperature (of the neutral prior to ionization), and this may be due to centrifugal effects (rotational energy) playing a role in the decomposition (*I38*). Kim and Cooks (*I26*) have discovered that the stereoisomers meso- and *d,l*-2,3-difluorobutane exhibit different metastable peak shapes for loss of HF. Another group active in these studies has been Holmes et al., who have been concerned with elucidating reaction processes and formulating mechanisms and ion structures from energy releases and accurate appearance potentials. They have reported energy releases for $(C_7H_{11})^+ \rightarrow (C_5H_7)^+$ (*I15*), $(C_3H_7)^+ \rightarrow (C_3H_5)^+$ (*I18*) and decompositions of $(C_3H_8)^+$ (*I17*); three distinct structures of formula $(C_2H_4O)^+$ have been proposed on the basis of differing metastable peak shapes (*I16*; see also *O33*). Energy releases in metastable decomposition of substituted 2,4-azetidinediones have been reported in a study concerned with analogies between EI and photochemistry (*I6*). This latter paper prompts the comment that correcting metastable peak shapes by subtracting the main beam width generally introduces more error than it removes; similarly subtracting the square of the main beam width from the square of the metastable peak width and taking the square root of the result is not always advisable (the latter is accurate for pure gaussian peaks) (*I1, I42*). Some translational energies determined for faster ($<10^{-6}$ s) decompositions have been reported (*I29, I36*).

The criterion of "metastable abundances" for competing reactions continues to find use in mechanistic studies, particularly in conjunction with specific isotopic labeling (*I5, I10, I12, I27, I33, I37, I39, I44, I45*). For example, with the exception of that from spiropentane, $(C_5H_8)^+$ molecular ions from various precursors show the same relative metastable abundances and, hence, probably decompose over the same energy surfaces at these times (*I14*). There has been a thorough study into the structures of $(C_2H_5O)^+$ ions formed variously, by dissociation of propan-2-ol and by ion–molecule reactions of acetaldehyde or ethylene oxide with $(H_3O)^+$ (*I24*). Ion kinetic energy (IKE) spectroscopy *per se* (i.e., with detector between electric and magnetic sectors) no longer seems to be an active field (*I34*). At present, the struggle for acceptance between the synonymous acronyms DADI and MIKES appears to be very much in the balance (*I19, I35, I37, I45*). The expert discussions of factors affecting the internal energy of ions *formed* by unimolecular ion decomposition draw heavily on metastable data (*I2, I31*).

Deuterium isotope effects have been determined for a number of metastable decompositions, often with a view to elucidating mechanisms (*I20, I28*). The isotope effects on loss of $H_2$(HD) from $CD_2CHD$, may be too large to explain even by invoking quantum mechanical tunneling (*I13*). It has been argued (*I21*) that, because metastable abundances $I_{m^*}$ for loss of $H_2$, HD, and $D_2$ from certain partially deuterated hydrocarbons follow the relationship $[I_{m^*(HD)}/I_{m^*(D_2)}]^2 = [I_{m^*(H_2)}/I_{m^*(D_2)}]$, the transition states for the processes are symmetrical. It has been pointed out that, given sufficient sensitivity and energy resolution, naturally occurring isotopes can be exploited for the study of isotope effects [e.g., in butane *m/e* 59 → *m/e* 42 represents $(^{13}CC_3H_{10})^+ \rightarrow (C_3H_6)^+ + {}^{13}CH_4$] (*I3*).

An interesting set of papers by Williams and Hvistendahl seeks to associate energy released in a metastable decompo-

sition with the orbital symmetry characteristics of the processes involved in the reaction. They have suggested that the relatively large discrete energy releases observed for the loss of $H_2$ from certain hydrocarbon ions reflect reverse activation energies arising from unfavorable orbital symmetries (i.e., processes are "forbidden" according to Woodward–Hoffman rules) (*I47, I48*). Similarly, large activation energies (200/300 kJ $mol^{-1}$) for 1,3-hydrogen shifts in oxonium ions are attributed to the processes being orbital symmetry "forbidden" (*I22*).

**Photoionization (PI).** The sort of precision achieved nowadays in photoionization (PI) is exemplified by ionization potentials of carbon dioxide (measured using synchrotron radiation) quoted at ±0.2 Å (±0.003 eV) (*J22*) and by measurements on oxygen at a resolution of 0.07 Å (*J13*).

An exciting development during the past two years has been the particular photoelectron/photoion (PE/PI) coincidence method of Baer et al. (*J32*), which allows *rate constants and translational energy releases for unimolecular (metastable) decomposition to be determined at selected internal energies.* Coincidences are measured only for photoelectrons with zero kinetic energy, so that the internal energy of the molecular ion is chosen by varying the photo energy. The metastable lifetimes of these energy-selected molecular ions, and the translational energy released during their decomposition, are measured using a time-of-flight method (*J26*). Ionization and appearance potentials are also obtained (*J29*). In the case of $(C_4H_6)^+$ decomposing to $(C_3H_3)^+$, the lifetimes decay exponentially with time as the quasi-equilibrium theory might predict (*J32*). However, for a number of other decompositions [loss of HCl from $(C_2H_3Cl)^+$ and $(CH_2ClCH_2Cl)^+$, loss of Cl from $(C_3H_3Cl)^+$, loss of Br from $(C_3H_3Br)^+$], lifetimes do *not* decay exponentially, indicative perhaps of more than one reaction channel contributing to each decomposition (*J4, J27*). The technique elegantly demonstrates how the translational energy release observed for a two-component decomposition changes according to the internal excitation energy (*J28*). Another photoelectron/photoion (PE/PI) study (*J15*) determined rate constants (in the $10^6$ $s^{-1}$ region) for decomposition of benzene and benzonitrile at selected internal excitation energies; one significant conclusion is that in earlier charge exchange experiments by Andlauer and Ottinger on the same reactions, the amount of translational energy converted to internal energy of the molecular ions was underestimated by a few tenths of an eV. These PI/PI measurements (*J15*) support the idea that there are two groups of noncompeting decompositions from ionized benzene (see also *J14*). Somewhat similar questions concerning energy deposition through charge exchange have been raised by a zero kinetic energy PE/PI coincidence study of $C_2H_4$ and $C_2D_4$ (*J24*). PE/PI measurements (*J23*) on hexafluoroethane suggest that loss of $F^\cdot$ occurs from an excited electronic state of $(C_2F_6)^+$, whereas formation of $(CF_3)^+$ involves only the ground state. Other coincidence studies have concerned acetone and dimethylmercury (*J17*) and $CF_4$, $N_2O$, and COS (*J6*); the mass resolution is very low in some of these measurements. Radiative lifetimes have been reported for some small ions (*J5, J18*).

Buttrill (*J7*) has resolved metastable lifetimes (50–200 μs) of molecular ions formed by PI, and suggests that there are three discrete states of $(C_7H_8)^+$ (from toluene) involved in the loss of H. This interpretation has been criticized (*J8, J19*). PI mass spectra have been reported for stereoisomeric cyclohexyl molecules (*J3*), amino acids and small peptides (*J20, J21*) and *trans*-azomethane (*J16*).

PI has been used to form ions in a particular electronic state with a *selected vibrational quantum number*, so that the ion–molecule reactions of the species can be measured at different vibrational energies (*J9, J10*). Thus, $(O_2)$ $(a^4\pi_u)$ + $O_2 \rightarrow (O_3)^+ + O$ proceeds only for vibrational quantum numbers $v = 5$–10 (*J12*); on the other hand, the reaction $(NO)^+ + i\text{-}C_4H_{10} \rightarrow HNO + (C_4H_9)^+$ shows little dependence on vibrational energy (from $v = 0$–4 (*J25*). Other PI studies have shown that the $(O_2)^+$ ion reacting with $N_2$ to form $(N_2O)^+$ is in an excited electronic state (*J2*); similarly, the $(O_2)^+$ ion reacting with $H_2$ to form $(HO_2)^+$ is electronically excited (*J1*). PI has been used to initiate clustering of $CH_3OH$ around $(NO)^+$ (*J30*), and to determine relative proton affinities of $H_2S$ and $CH_3OH$ (*J30, J31*). Ion-molecule reactions of allylamine (*J33*) and cyclohexane (*J11*) have been investigated by PI.

**Unimolecular Rate Theory.** During the past few years, there have been developments in unimolecular rate theory which hold significance for mass spectrometry. We refer to the pulsed laser/fluorescence experiments, and the theoretical treatments stimulated by these measurements, which suggest that vibronic relaxation in isolated molecules need not be fast and can indeed be rather slow (*K2, K4* and references therein, *K6, K14, K15*). For example, rate constants for intersystem crossing in ketones (singlet → triplet), which is faster than internal conversion, are of the order of $10^9$ $s^{-1}$ (*K3*). Rice et al. (*K5*) have proposed that internal conversion in styrene puts energy into torsional modes which lose this energy only very slowly, so that vibronic relaxation is not complete prior to cis–trans isomerization in $10^{-8}$ s. Pocius and Yardley (*K11*) have experimentally verified that there can be vibrational modes of an isolated molecule which play no part in radiationless decay. These various studies, while not specifically concerned with mass spectrometry, do combine to throw strong suspicion, particularly at low excitation energies, on the general validity of the quasi-equilibrium theories' (QET) assumption of energy randomization prior to chemical reaction. Such suspicions are reenforced by chemical activation studies of Rabinovitch et al. (*K8, K12*), who conclude that energy randomization is not complete within a picosecond in certain molecules.

A quantum ergodic theory of unimolecular reaction, which is still being developed, precludes assumptions of energy randomization (*K9, K10* and references therein). Alexandru (*K1*) has published a further theoretical paper on ion fragmentation. A review of unimolecular reactions contains some interesting points (*K7*). The discussion of approximations used for hindered internal rotations in energy level sums is useful for practical applications of QET (*K13*).

**Molecular Orbital (MO) Calculation.** Molecular orbital (MO) calculations are of interest to the mass spectrometrist because, in principle, they identify stable ion structures and provide information on geometries and energies which is not available from experiment. Thus they ought to complement mass spectrometry experiments (e.g., CID, ICR) where identification of structure rests upon inference from chemical reactivity. In practice, it can be difficult to evaluate the reliability of a particular calculation. The clear appraisal of the different MO methods given by McMaster (*L30*) could be useful in this respect, and MO calculations of carbocations have recently been reviewed by Hehre (*L16*). It had been often suggested that semi-empirical methods tended to overestimate stabilities of nonclassical ions (relative to those of their classical isomers); however, Dewar et al. (*L2*) claim that this deficiency has been overcome by their MINDO/3 method. On the other hand, MINDO/3 has been unfavorably compared to *ab initio* methods by Pople (*L34*) and Hehre (*L18*), although this implied criticism has been refuted by Dewar (*L11*).

Organic polyatomic ions treated by *ab initio* methods during the past two years include acetyl cations (*L35, L40*); haloethyl cations (*L20*); acyloxycations (*L29*); $(C_4H_7)^+$ (*L19*); $(C_3H_7)^+$ (*L14*); protonated amines (*L21*); $(HCHO)^+$ and $(HCHO)^-$ (*L8, L32*); $(CH_3)^-$, $(C_2H)^-$, $(C_2H_3)^-$, and $(C_2H_5)^-$ (*L39*); $(NO_2)^+$ and $(CO_2H)^+$ (*L5*); $(CH_5)^+$ and $(CH_5)^-$ (*L12*); $(C_6H_9)^+$ (*L15*); $(CH_2SH)^-$ (*L37*); $(C_2H_2)^+$ and $(C_2H_2)^-$ (*L4*) and the tetracyanoquinodimethane anion and cation (*L24*). The interconversion of cyclopropyl and allyl structures has been treated using configurational interaction for the cations, anions, and radicals (*L31*). There have been valence bond calculations of $(C_5H_5)^+$, $(C_5H_5)^-$, $(C_7H_7)^+$, and $(C_7H_7)^-$ (*L13*).

Semi- or non-empirical MO methods have been applied to acyloxy and dioxacyclopropyl cations (*L36*); $(CH_2OH)^+$ and $(CH_2SH)^+$ (*L1*); $(C_2H_2SH)^+$ (*L6*); $(C_2H_2F)^+$ (*L7*); and $(CH_2NH)^+$, $(CH(NH_2)_2)^+$, and $C(NH_2)_3)^+$ (*L26*). Stabilization of cations by σ-delocalization has been discussed (*L38*).

MO calculations are also quite commonly made with the object of rationalizing mass spectra (*L22*). The CNDO/2 calculation of a partial energy surface of the ethylamine ion falls in this category (*L27*). There has been a series of papers seeking to elucidate specific ion reactions by means of semi-empirical MO calculations (*L3, L25, L33*); the value of this work hinges upon the accuracy of the calculations and this is very difficult to estimate. Ion decomposition following charge exchange with high energy incident ions in a tandem mass

spectrometer has been rationalized using MO calculations, on the grounds that fragmentation occurs at the bond from which the electron is removed (*L23, L41*). This type of explanation is open to criticism (*L30*).

Some of the recent MO work on orbital and state symmetry and correlation is relevant to mass spectrometry (*L10, L17, L28*), now that attempts are being made to relate activation energies of gaseous ionic processes to Woodward–Hoffman Rules (see *I22*). We draw attention to the situation known as "subjacent orbital control", where the energy of the transition state in the route "forbidden" by orbital symmetry is *lower* than that in the "allowed" route, because of orbitals below the highest occupied MO's playing a dominant role (*L9*).

**Negative Ions.** Mass spectrometry of negative polyatomic ions has been recently reviewed by Bowie and Williams (*M7*). An earlier more physically inclined review is entitled "gaseous negative ions" (*M16*; see also *M8*). Negative ion–molecule reactions are currently attracting a good deal of interest particularly in chemical ionization (see sections on ion–molecule reactions). A novel method of measuring ion–molecule processes which would lend itself to adaptation for use with commercial mass spectrometers has been described (*M27*).

Work continues toward developing negative ion mass spectra produced by electron impact (*EI*) at 70 eV for analytical purposes (*M2, M6, M17, M37*). These spectra are due to secondary electrons, and thus are suppressed by the introduction of $SF_6$ as a thermal electron scavenger (*M3*). Discussion of these spectra embraces familiar mechanisms (such as the retro Diels–Alder) (*M5*), substituent effects, and isotopic randomization (*M4*).

Ionization efficiency curves continue to be measured by EI for a variety of compound-types (*M19, M32, M33*). It has been suggested that thermal emission of negative ions from the hot filament can compromise this type of study (*M15*). Monoenergetic electron beams have been used to study dissociative capture in small molecules (*M29, M39*). The angular distribution of $(O)^-$ produced through dissociative ion–pair formation in $O_2$ has been measured (*M34, M35*), and ion-pair formation in $CF_4$ has been studied by a coincidence technique (*M1*). Sharp resonances seen in electron transmission spectroscopy of benzene and *N*-heterocyclics represent temporary negative ions (*M26*). Translational energies of ions formed by dissociative resonance capture are measured as a function of excess energy by Franklin et al., and provide important information concerning energy partitioning (*M18, M36*).

Electron swarm methods provide information on electron attachment processes (*M11*), and have been used to study clustering in water (*M38*). It has been suggested that benzene has a small but positive electron affinity (*M10*). Cesium collision studies produce negative ions by charge exchange between incident cesium atoms (with translational energies varied between 0 and 40 eV and higher) and the thermal gaseous sample, e.g., $Cs + m \rightarrow (Cs)^+ + (m)^-$ (*M31, M25*); the threshold for charge exchange reflects the electron affinity. Fragmentation patterns are produced for polyatomic samples and bond energies can be estimated. The past two years have seen the technique applied to both polyatomic organic molecules (benzoquinone, maleic anhydride) (*M12–14*) and small inorganic molecules ($O_3$, $SO_2$) (*M28*). Collisions between organic molecules and rare gas atoms in Rydberg states produce negative organic ions (*M30*).

Tunable lasers are now quite commonly used for photodetachment studies, and provide good values for electron affinities (*M20, M21*). Fixed frequency lasers demand that the energy of the ejected photoelectron be analyzed (*M9*). Surface ionization has been used to study photodetachment from $[(CN)_2C{=}C(CN)_2]^-$ (*M22*). There has been a report of photodissociation of a negative ion (*M24*; see also *M23*).

**Field Ionization (FI) and Field Desorption (FD).** Field ionization (FI) in general has been reviewed by Robertson (*N33*), and field desorption of organic compounds has been reviewed by Beckey and Schulten (*N11, N12, N43, N44*). A new edition of Beckey's book is in preparation (*N9*), and the relative merits for analytical purposes of FI, FD, chemical ionization, and electron impact have been evaluated (*N15, P40*). The crucial feature of an FI source remains the emitter; however, it is probably safe to say that conditioning of tungsten W wires is now routine in many laboratories [notably Beckey's laboratory (*N2*)]. A useful calibration curve of wire heating current vs. emitter temperature has been given (*N25*). A pre-roughing treatment is claimed to facilitate conditioning of W wires (*N8*). An electrochemical method of generating metal dendrites for use as FI emitters has been described (*N52*), and the use of etched foils as emitters has again been advocated (*N7*). A small bundle of short thin (10 $\mu$m) W wires performs effectively as a multitip emitter, and has the appropriate symmetry for coupling with a quadrupole mass spectrometer (*N10*). The multitip array emitter (*N4, N50*) produced by vapor deposition was covered in the previous review (*B4*). The volcano FI source shows promise for higher routine sensitivity (Aberth, Wilder, and Burlingame, unpublished results). The production of negative ions by FI has been achieved using a $\frac{1}{16}$-inch W rod which is simply broken to produce a surface sufficiently rough to emit ions (*N5*). Similar experiments have been reported using a multitip array (*N6*). Quite possibly negative FI will be useful for analytical purposes and it does hold fundamental interest. However, it is totally incorrect to claim, as these authors do (*N6*), that negative FI has not been described before. Negative FI was studied extensively by Robertson and Williams in the early 1960's, and has been reported in the open literature by them (*N34*; see *N53* for a full discussion of the whole subject of negative FI) and by other workers (*N1*). Further, these recent workers (*N5, N6*) report that negative ions are formed below the field threshold for field emission of electrons; this is contrary to the findings of the earlier investigation (*N34, N53*).

Field desorption (FD), meaning the technique in which a solution of sample is placed on the emitter before introducing the emitter into the vacuum (*N32*), is *sine qua non* the method of choice for mass spectrometric analysis of nonvolatile thermally unstable compounds. However, this is not to say that FD is yet an established tool of the analytical chemist. The ground rules for interpretation of mass spectra obtained under FD conditions are still being laid (*N45*), and the majority of reported spectra are still of "compounds from the bottle." It cannot be assumed *a priori* that the base peak in an FD mass spectrum is a molecular ion [or $(M + 1)^+$]. The FD mass spectra of organic and inorganic salts often exhibit no molecular ion at all, although there tend to be cluster ions [e.g., $(M + Na)^+$, $(M + 2Na)^+$] which provide a clue as to the molecular weight (*N16, N26, N47, N48*). In the FD mass spectra of onium salts (ammonium, phosphonium, etc.) the cation is usually the base peak (*N41*; see also *N55*). Generally speaking, a small amount of a metal cation on the FD emitter tends to have an effect on the spectra quite out of proportion to its abundance. Adding a macrocyclic ligand to the sample solution has been suggested as a ploy for producing smooth reproducible spectra despite the presence of alkali metal cations (*N54*; see also *N20*). Alternatively, cationization can be encouraged, so as to obtain a strong $(M + \text{cation})^+$ peak from which to calculate the molecular weight; three methods designed to ensure cationization have been described (*N39*). It also cannot be assumed *a priori* that a FD mass spectrum will contain no "fragment" ions; sometimes such a moiety is the base peak (see for example *N15*). So-called field desorption mass spectra can contain ions resulting from several different physical processes such as field ionization, surface reactions, pyrolysis moieties, etc., and the source operating conditions which produce these phenomena are not yet well understood. Quadrupoles offer a fast sweep time (but poor mass resolution) which is an advantage for FD (*N17*), and inclining the analyzer at an angle to the source reduces noise to an acceptable level (*N22*). Accurate mass measurement in high resolution FD is possible through peak matching (*N30*), as well as with photoplates.

FD mass spectra of specific compounds are covered in the applications sections. The list of compounds for which FD spectra have been obtained includes oligosaccharides (*N31*; see also section on sugars), cyclophosphamides (*N42*; see also section on pharmacology), glycosides (*N28, N46*; see also section on complex lipids); aerosols from ozonolysis of but-1-ene (*N49*; see also section on environmental chemistry).

There seems to have been something of a resurgence of interest in the measurement of FI appearance potentials (AP's) (*N18, N21, N23*); the FI AP is the minimum energy needed to be supplied by the field to produce a particular ion. Their values are derived from the measured translational energy distributions of the ions in question. The AP's for some fragment ions confirm that many field-induced reactions require little activation energy (*N23*). The doubly-charged ions ob-

served in FI commonly arise through ionization of a chemisorbed molecule which loses a second electron in being desorbed from the surface (*N36*; see also *N14*). The AP for $(C_6H_6)^{2+}$ from benzene is too low for the species to have an intact cyclic structure (*N37*). A study of surface processes (see also *N35*) concludes that surface hydrogen rearrangements in molecular ions are *intermolecular* and not *intramolecular*, provided the ions are not chemisorbed (*N38*). Adsorption of hydrogen mixtures on FI emitters has been investigated (*N40*). A number of papers have been concerned with FI of inorganic compounds such as sulfur (*N13*), perchloric acid (*N51*), and boron hydrides (*N27*).

A theoretical treatment of field dissociation calculates finite probabilities of transitions to vibrationally excited states, although mentioning that the presence of the surface tends to encourage adiabatic transitions (*N24*). There has also been a thorough theoretical study of field dissociation of $H_2$ and HD (*N19*). Using a CNDO method, a Russian group has calculated the electronic structures of acetaldehyde and propanal in a $10^{10}$ V m$^{-1}$ field (*N3, N29*).

**Collision-Induced Decomposition (CID).** Interactions between ions of high velocity (typically 1–10 keV) and thermal neutrals can be studied using commercial mass spectrometers [perhaps slightly modified (*O4*)] and conventional techniques (*B4*). The types of processes induced through such interactions include charge stripping [$(m)^+ + N \rightarrow (m)^{2+} + N + e$] (*O15*) and charge inversion of both negative [$(m)^- + N \rightarrow (m)^+ + N + 2e$] (*O9, O11*) and positive ions [$(m)^+ + N \rightarrow (m)^- + (N)^{2+}$ *and* $(m)^+ + N \rightarrow m + (N)^+$ followed by $m + N \rightarrow (m)^- + (N)^+$] (*O1, O20*). There has been a detailed study of the charge exchange $(m)^{2+} + N \rightarrow (m)^+ + (N)^+$ in rare gases (*O2*; see also *O5, O32*). However, the most frequently studied type of process remains collision-induced decomposition (CID), in which the incident ion retains its charge but gains internal energy and decomposes (*O16, O21*). It has also been pointed out that rather similar decomposition can be induced (sometimes inadvertently) by collision of ions with metal surfaces (e.g., walls of the analyzer) (*O14, O17*).

Collision-induced decomposition (CID) is an important method for characterizing stable ion structures, and as such has been widely applied by McLafferty et al. They use a reverse geometry instrument (*B4*), and refer to their experiments as "collisional activation (CA)". A number of stable $(C_7H_7)^+$ structures (tropyllium, benzyl, *o*-, *m*- and *p*-tolyl, norbornadienyl) have been distinguished by this method (*O29*), also a handful of $(C_3H_6O)^+$ structures (*O35*) and three stable $(C_2H_4O)^+$ structures ($CH_2CH_2O$, $CH_3CHO$, $CH_2{=}CHOH$) (*O34*; see also *I16* and *O19*). Other ions investigated in this way include oligopeptides (*O28*), $(C_8H_9)^+$ (*O30*), $(C_{12}H_{12}O)^+$ and $(C_{12}H_9O)^+$ (*O26*), $(C_2H_6N)^+$ and $(C_3H_8N)^+$ (*O25*), $(C_9H_{11}O)^+$ (*O31*), and the tetramethylenechloronium ion (*O33*). Bowie (*O7, O8, O10*) has explored the possibilities for determining negative ion structures through CID. Ion structure studies have also been reported by Levsen et al. (*O6, O22, O23, O27*); in particular, we note the investigation of $(C_7H_8)^+$ and $(C_8H_8)^+$ produced by field ionization (FI) (*O24*). In FI studies where the interest lies in unimolecular metastables, it can be difficult to avoid collisional contributions to metastable peaks. Presumably this is because in FI the number of stable ions tends to be high relative to the number of ions with internal energies such that they decompose unimolecularly in the field-free regions (see *G10*).

Using a longitudinal mass spectrometer and a range of collision gases (He, Ne, Ar, Kr, Xe), there has been a careful determination of isotope effects in the collision-induced formation of methyl ions $[C(H,D)_3]^+$ from $[C(H,D)_4]^+$ (all five isotopic varieties) (*O13*). The CID of $(H_2)^+$ following *vibrational* excitation has been treated theoretically (*O18*). Light in the wavelength range 300–650 nm is emitted from both excited ionic states and Rydberg states following collision of mono- and diatomic ions at (500–5000 eV) with $CO_2$ (*O12*). The photoionization instrument of Baer et al. (see *J32*) has been used to study CID of $(CH_2Br_2)^+$ in selected internal energy states (*O3*).

**Chemical Ionization.** For the purposes of this review, we loosely define chemical ionization (CI) as experiments in which a sample is mixed with an excess of reagent gas and the reagent gas is ionized, initiating ion–molecule reactions through which the sample itself is eventually ionized and subsequently analyzed mass spectrometrically. Chemical ionization has matured quickly, is extremely widely applied (*P7, P44, P45, P52*, and Applications Sections) and is frequently reviewed (*P30, P37, P40, P48, P51*).

Chemical ionization sources which operate at or close to atmospheric pressure represent one of the most exciting developments in mass spectrometry during the past two years. The atmospheric pressure ionization (API) of Horning et al. (*P19*) uses either electrons from $^{63}Ni$ or a corona discharge to ionize a gas stream (often $N_2$) containing the sample. The ion–molecule reactions induced in turn ionize the sample, and ions are extracted continuously through a pinhole (25 $\mu$m). The technique is directly related to the plasma chromatograph (*P30–34*) with the difference that API uses a quadrupole to analyze the extracted ions. Plasma chromatography relies on drift times along a tube ("ion mobility spectra") to achieve mass analysis (*P5*). With the API source, it is probably possible to ionize almost 100% of the sample. However, the extraction efficiency in terms of the number of ions passing through the pinhole is probably only in the region of 1%, in addition to which, the extracted ions diverge from the pinhole so that a further proportion is lost prior to mass analysis and detection. Yet, despite these losses, the sensitivity of API is at the subpicogram level (*P6*) At these sensitivity levels, traces of water in the carrier gas are a problem since they may be ionized in preference to the sample (depending on the relative proton affinities). In common with other CI techniques, API provides both negative and positive ion mass spectra (*P9, P10*). Coupling of API with liquid chromatographs has been described (*P17, P18*; see section on GC/MS Computer Techniques). Specific applications of API are covered in the later sections of this review. Gray (*P12, P13*) has developed an atomospheric pressure ionization source which operates at high temperatures (core temperature 5000 K) and can be used for elemental analysis (e.g., of aqueous solution of cobalt and lead salts).

Hunt et al. (*P23*) have used Townsend discharge in CI at the more usual operating pressures (1 Torr), thereby avoiding the sort of problems encountered when a hot filament is exposed to reagent gases with oxidizing properties. The same group has described the use of oxygen as a reagent gas to produce negative ions (*P22*; see also *P34*). Methylene chloride has also been used as a reagent gas for negative CI mass spectra, producing ions by chloride attachment (*P46*). Reagent gases for positive CI mass spectra are better documented than those for negative CI, but there has still been a considerable amount of work in this area (*P28, P53*). There are advantages to using nitric oxide and nitrogen mixtures as the reagent gas for biologically significant molecules because $(NO)^+$ gives a molecular ion and $(N_2)^+$ produces a fragmentation pattern (*P27*). 1,2-Diaminoethane and 2-aminoethane and 2-aminoethanol can modify the reactivity of an isobutane plasma to advantage (*P3*). Nitric oxide reagent gas has given good results with aldehydes (*P25*) and with morphine and tropane alkaloids (*P24*; see also *P20, P21*, and section on Pharmacology). Hydrogen has been used for certain explosives (*P11*), an ammonia/isobutane mixture for oligosaccharide peracetates (*P8*), and methane, propane, and hydrogen for certain steroids (*P39*). Some chemical mass markers for CI have been suggested (*P2*). Solutions of organic samples (1 in $10^6$ level) can in favorable circumstances be injected directly into the heated inlet system of a CI source (*P43*). An ingenious variation has been to generate water as a reagent gas in a solid sample probe by heating inorganic salts (*P4*).

Meisels et al. (*P38*) have shown that the arrival times (reflecting source residence times) of $(H_3O)^+$, $(H_5O_2)^+$, and $(H_7O_3)^+$ in CI of water differ, indicating that the reversible reactions forming these ions do not lie at equilibrium. However, the reactions appeared to be pressure-independent and yielded linear van't Hoff plots. The conclusion drawn is that *linear van't Hoff plots and pressure independence do not indicate that a reversible reaction in a CI source lies at equilibrium*. The temperature dependence of $(CH_4D)^+ + CH_4 \rightarrow CH_3D + (CH_5)^+$ has been investigated down to temperatures as low as 80 K; the process in fact appears to be temperature-independent, consistent with a zero activation energy (*P42*). Arrival time distributions have been reported for negative ions from CI of $CO_2$ (*P41*).

Some mechanistic aspects of CI of esters have been elucidated by Munson et al. (*P26*) using $^2H$-labeling. The major ions in the isobutane CI spectra of secondary alcohols can be

accounted for by a long-lived $(M + 57)^+$ ion (*P29*). Other mechanistic studies (*P16, P36*) have reported on stereospecific loss of water from bicyclic ketones (*P1*), intramolecular hydrogen bonding in bifunctional molecules (*P50*), ammonolysis of base-sensitive bonds (*P14*) and *tert*-butyl compounds (*P35*). CI of the epoxide determines the position of an olefin bond in an aliphatic chain (*P47*). A study of fluorotoluenes demonstrates the usefulness of perdeuterated reagent gases for elucidating reaction pathways (*P15*).

**High Pressure Mass Spectrometry (HPMS).** High pressure mass spectrometry (HPMS) covers experiments in which ion–molecule reactions are induced in the ion source of the mass spectrometer and ions continuously or intermittently are extracted for analysis (*Q5, Q12*). Theoretical papers of general significance are dealt with here; chemical ionization, however, is discussed separately.

Determination of gas-phase equilibrium constants remains an active concern in HPMS, although there is discussion concerning the reliability of the results (*R75, T20*). Kebarle et al. have reported a large number of precise measurements of gas-phase acidities $[(A_1)^- + A_2H \rightleftharpoons A_1H + (A_1)^-]$ (*Q16, Q33, Q34*). They have also reported on clustering in methane (*Q7*), the proton affinity of propane (*Q6*) and the clustering reaction $H_2 + (H_n)^+ \rightleftharpoons (H_{n+2})^+$ (up to $n = 9$) (*Q8*). Equilibrium measurements extending to low temperatures have been reported from Poland (*Q13, Q35*; see also *Q14*). Field et al. have studied clustering in amines (*Q18*), tertiary alkyl carbonium ion stabilities (*Q30*), and several association reactions of the type likely to occur in the atmosphere (*Q19*), and there has been an investigation of the gas-phase hydration of $(Bi)^+$ (*Q32*).

Harrison et al. have been active in the field of ion–molecule reactions, using the technique in which ions are trapped perhaps for milliseconds in the space charge of an electron beam (see also *Q24*) together with extensive isotopic labeling of reactants. Among the systems measured are 2-methylpropene (*Q1*), propane and methane/propane mixtures (*Q29*), thiols (*Q27, Q28*) and reactions of $(C_2H_5)^+$ derived from various precursors (*Q29*). Relative efficiencies of different bath gases for collisionally stabilizing excited $(C_5H_9)^+$ in the ethylene system have been determined, and the conclusion reached is that stabilization involves long-lived complexes (*Q22*). Energy redistribution involves transitional rather than vibrational modes of the bath gas (*Q22*). The temperature dependence of ion–molecule reactions has been the subject of recent discussion (*Q17*, see also *P38*), and a new explanation has been put forward for the negative dependence of certain slow reactions (*Q20*). The reaction $(C_2H_5)^+ + CH_4 \rightarrow (C_3H_7)^+ + H_2$ shows a linear positive dependence on temperature over the range 250–650 K (*Q9*), and $(H_3)^+ + 2H_2 \rightarrow (H_5)^+ + H_2$ shows a negative dependence (usual for termolecular process) (*Q10*). A series of papers on SN2-type association reactions has sought to determine the role of solvation in the analogous solution reactions (*Q2–4*). There are apparently two distinct dimers $[(C_6H_6)_2]^+$ of benzene (*Q11*; see also *R3*). Using three pulses instead of the usual two in pulsed HPMS has, it is claimed, significant advantages for determining the energy dependence of ion–molecule reaction rates (*Q25*). A new method of trapping ions has been described (*Q21*).

Su and Bowers (*Q31*) have extended their theory of ion–molecule reactions in polar molecules to cope with quadrupole moments. A criticism has appeared of those experiments using "field-free" ion sources to determine thermal reaction rates; it is suggested that the thermal velocity distribution must be taken into account in interpreting the attenuation results (*Q15*). The conversion of phenomenological to microscopic cross sections has been discussed (*Q23*).

**Ion Cyclotron Resonance (ICR).** Ion cyclotron resonance (ICR) is one of the most active areas of mass spectrometry, perhaps because its unique capabilities for ion–molecule studies (*B4*) are combined with a ready commercial availability. A major theme of ICR work continues to be determination of equilibrium constants of ionic gas-phase reactions; the concern is generally with relative (rather than absolute) values for a series of reactions. The gas-phase equilibrium constants are considered to reflect intrinsic chemistry, while differences between them and the equilibrium constants for the corresponding reaction in solution are attributed to solvation. Perhaps it is an indication that these gas-phase measurements are gaining acceptance in physical organic chemistry, when measurements of acidities in DMSO are undertaken with a view to comparing the results with *literature* gas-phase data (rather than *vice versa*) (*R12*). Staley and Beauchamp (*R74*) have addressed the key question of whether the gas-phase values of equilibrium constants are reliable (there is always a lingering suspicion that the reversible reaction may not lie at equilibrium) by comparing the results for the reaction $(CO_2H)^+ + CH_4 \rightleftharpoons (CH_5)^+ + CO_2$ obtained by different techniques, viz., ICR, flowing-afterglow, high pressure mass spectrometry, and the trapping of ions in the space charge of an electron beam. The values from ICR and flowing-afterglow agree (see also *T8*) and are higher than those from the other two techniques (which also disagree with each other); the conclusion drawn (*R74*) is that the results from these other two techniques are unreliable and do not reflect equilibrium conditions. It should, however, be noted that results from high pressure mass spectrometry for clustering of $NH_3$ about $(NH_4)^+$ do agree with the results from a number of experiments (including flowing afterglow) in which equilibrium is probably attained (*T20*; see also *R8*).

ICR equilibrium measurements (*R37*) have shown that, in the gas-phase, the stabilizing effects of para-alkyl groups on protonated benzene follow the order Me < Et < *i*-Pr < *t*-Bu rather than the Baker–Nathan order observed in superacid solution. Stabilities of carbocations (*R82, R85*), fluorocarbonium ions (*R19*), and alkoxide ions (*R6, R7*) have been investigated by ICR with a view to elucidating solvation effects. The gas-phase basicity of manxine, when considered together with its photoelectron spectrum, suggests a planar bridgehead in both the neutral and the radical-cation (*R10*). Other types of solution process simulated in the gas-phase and studied by ICR include acetylation of cresols (*R22*, see also *R21*), aromatic nucleophilic reactions (*R20*), esterification (*R76*), nucleophilic substitution at carbonyl centers (*R9, R14, R16*), base catalyzed eliminations (*R68*) and intramolecular hydrogen transfers of carbonium ions (*R45*). Unimolecular decompositions and ion–molecule reactions of bifunctional ethers have been measured to pursue the analogy between intramolecular rearrangement and bimolecular processes (*R57*). Interestingly, hydrogen randomization appears to occur in protonated benzene (*R34*). Inorganic chemistry has seen ICR investigations of the gas-phase ion chemistry of iron complexes (*R31, R32*), chromium complexes (*R30*), phosphines (*R73, R79, R80*), organoboron compounds (*R58*) and reactions of alkali ions with organic molecules (*R81*).

There have been a large number of papers concerned more traditionally with delineating and determining rate constants for ion-molecule reaction pathways in various gases [*tert*-butyl alcohol (*R11*), organic cyanides (*R15*, see also *R17, R18, R84*), thiocyanates (*R53*), formaldehyde (*R41*, see also *R42*), mixtures of small molecules (*R39, R40, R44, R47, R52*)]. In particular, there has been a series on fluoroethylenes (*R1–3*, see also *R67*); the same group has tested their average-dipole theory on reactions of $(Cl)^-$ with dichloroethylene and difluorobenzene (*R75*). $(N_2)^+$ has been produced in an excited electronic state and its ion–molecule reactions measured (*R13*). Hydrogen atom abstractions envisaged to occur in interstellar clouds have been investigated (*R43*). Photoionization has been used to initiate ion–molecule reactions of ethylene in an ICR cell (*R49*).

Several workers have used ICR to study chemical ionization (CI), in particular elucidating protonation in esters (*R59*) and properties of NO reagent gas (*R83*). $(CHF_2)^+$ has been examined as a possible reagent gas (*R78*). Charge exchange cross sections have been determined by ICR (*R48*). By trapping ions in an ICR cell for seconds, it is possible to use CI to detect vapors at pressures as low as $10^{-10}$ Torr (*R56*). Another novel type of experiment possible through ion trapping allows detection of the *neutral* products from ion–molecule reactions (*R50*).

ICR continues to be used to characterize ion structures through their ion–molecule reactivity, and ions studied in this way include $(C_4H_8O)^+$ (*R35*), cyclopropyl species (*R36*), $(CH_5)^+$ (*R69*), and $(SiH_5)^+$ (*R70*, see also *R54*). Stereoisomers have been distinguished (*R38*), as have the tautomeric $[(CH_3)_2N{=}CH_2]^+$ and $(CH_3NH{=}CHCH_3)^+$ (*R77*). It has been proposed that there are two $(C_7H_7)^+$ ions formed by loss of $H^\cdot$ from toluene. One undergoes ion–molecule reaction with toluene and is said to have the benzyl structure, while the other does not react with toluene and is said to have the tro-

pyrilium structure (*R27, R71*).

Photodetachment is conveniently studied in an ICR cell by trapping the negative ions for periods of seconds. Cross sections can be determined, and upper limits set on electron affinities (*R60–66*). Information can be gained regarding negative ion structures (*R61*). Photodissociation also continues to be studied using trapped ion ICR techniques [benzene (*R29*)/perfluoropropylene (*R33*)]. Photolysis of toluene ions has been performed with a trapped ICR cell (*R46*).

Fourier transform ICR represents an important instrumental development, which will improve the mass resolution of ICR and reduce sweep times (*R23–26, R51, R55*; see also section on Innovative Techniques and Instrumentation). The desirability of quantitative double resonance for complex reaction systems has been reemphasized (*R28*). A further theoretical treatment of power absorption has been put forward (*R5*). Possible pitfalls in interpreting pulsed ion ejection spectra have been emphasized by two recent papers (*R4, R72*) which show that certain reaction pathways proposed on the basis of such spectra in earlier papers are incorrect. It is suggested that noise may couple the electron impact spectrum with a pulsed ion ejection spectrum via space charge (*R72*).

**Tandem Mass Spectrometers and Beams.** Tandem mass spectrometers and beam machines remain the domain of the instrument builder, and studies of polyatomic systems with these instruments are still relatively rare. A commercial double-focusing mass spectrometer with a collision region between the sectors could be regarded as a longitudinal tandem mass spectrometer with high energy incident ions, but we consider such experiments separately (see section on Collision-Induced Decomposition). Beam studies tend to concern matters beyond the scope of this review, such as the large inelastic scattering of $(Na)^+$ by $D_2$ (*S3*), or energetics of charge transfer between $(Ar)^+$ and $H_2$ (*S14*).

A beam instrument, referred to as a chemical accelerator, which allows the ion gun to be rotated around the collision chamber, has been used to study the reaction dynamics of the process $(Ar)^+ + CH_4 \rightarrow (ArH)^+ + CH_3$ (*S20*). The interesting conclusion is that there is a translational energy threshold (0.1–0.2 eV) for this exoergic (~1.7 eV) process, thereby seemingly establishing an exception to the long-established maxim that exoergic ion–molecule reactions have no activation energy (*S19*). Lampe et al. (*S2, S9, S11, S12*) have investigated ion–molecule processes in silanes and silane/hydrocarbon mixtures using a longitudinal tandem mass spectrometer composed of two quadrupoles. They conclude that hydride transfers in monosilane and methylsilane occur via "direct stripping" at high energies, but via collision complexes at low energies (*S8, S10*). Another novel tandem instrument couples a Dempster magnetic sector with an ICR cell (*S15*) and has provided good results for reactions of $(CH_3)^+$ with small hydrocarbons (*S4*, see also *R72*).

The isotopically mixed products from the process $(CH_2)^+ + CD_4 \rightarrow (C_2(H,D)_5)^+ + (H,D)_2$ have been explained by postulating three separate reaction channels, none of which involve an intermediate (collision complex) (*S5*). Similarly, crossed beam measurements, using the instrument referred to as EVA, suggest that the process $(CH_3)^+ + C_2H_4 \rightarrow (C_2H_3)^+ + CH_4$ occurs via a direct mechanism despite showing isotopic "scrambling" (both D and $^{13}C$) (*S18*). The important point emphasized by these studies is that isotopic "scrambling" in an ion–molecule reaction does not necessarily mean that the process involves a long-lived intermediate or collision complex. The EVA instrument has been used for other work (*S17*), in particular a study of the process $(O)^+ + N_2 \rightarrow (NO)^+ + N$, believed to be one of the most important reactions in the F layer of the upper atmosphere (*S16*). Tandem mass spectrometers have been used to study isotope effects on charge exchange in methane (*S1*), energy transfer in charge exchange in methane (*S13*) and propane (*S7*) and fragmentation of thiols (*S6*). Some studies with longitudinal tandem instruments are covered in the section on Collision-Induced Decomposition.

**Flowing Afterglow and Drift Tubes.** Flowing afterglow is probably the technique of choice for thermal ion–molecule processes, and two groups actively engaged in such studies have recently reviewed their own work (*T2, T19*). Equilibrium constants determined in flowing-afterglow experiments have been found to agree with those from ion cyclotron resonance (ICR) and drift tube experiments (*T7*). The technique has been extensively applied to reactions of geo- and astrophysical interest (*T4*), such as clustering of ozone around $(O_2)^+$ and $(NO)^+$ (*T3*) and reactions of negative ions found in the lower atmosphere (*T5*). Other types of process investigated in flowing-afterglow experiments include proton transfer to ammonia (*T10*), reactions of $(N_2H)^+$, $(N_4)^+$ and $(N_3)^+$ with water (*T1*) and the reaction of $(NH_3)^+$ with hydrogen (*T8*) (which is slow at thermal energies but shows a *strong* energy dependence). It was also possible using this technique to study the gas-phase ion chemistry of nitric acid (*T6*).

There are various other types of experiment using drift tubes in which ions move through the gas under the influence of a small electric field. Products are analyzed by extraction into a mass spectrometer or by measuring drift times (mobilities) (*T13, T18*). Drift tubes have been employed to measure clustering in CO (*T11*), and clustering of various small molecules around $(NO)^+$ (reactions important in D region of atmosphere) (*T9*). Another reaction $(NO)^+ + 2N_2 \rightleftharpoons (NO\ N_2)^+ + N_2$, important in D region chemistry, has been studied in a drift tube (*T12*). Results for clustering of ammonia about $(NH_4)^+$ agree well with those from other techniques (*T20*) (see section on ICR). Results from a recently constructed *flow* drift tube (*T14, T16*) suggest that the internal (vibrational) energy distribution of ions in drift tubes can be substantially removed from equilibrium (*T17*). This instrument has been used to study reactions of $(H_2O_2)^+$, a species which occurs in the atmosphere at altitudes as high as 80 km (*T15*).

## APPLICATIONS IN BIOCHEMISTRY AND MEDICINE

**Amino Acids, Peptides, and Sequencing.** Multiple ion monitoring (MIM) has been developed for routine determinations of 12 amino acids isolated from biological fluids (*U35*); the acids were analyzed as their *n*-butyl ester/(*n*-Bu) *N*-trifluoroacetyl (N-TFA) derivatives using deuterated amino acids as internal standards for quantitation. A similar system is reported by Schulman and Abramson (*U34*) who evaluated both *n*-Bu/*N*-TFA and *N*-neopentylidine/*n*-butyl ester/trimethylsilyl ether derivatives. However, these authors favor the use of repetitive scanning operation over multiple ion monitoring (MIM) for greater flexibility even though sensitivity is reduced.

Single ion monitoring (SIM) of masses characteristic of certain functional groups has been used for the detection of trimethylsilyl (TMS) derivatives of primary amines [R–$CH_2$–$NH_2$] and α-amino acids [R–CH($NH_2$)–$CO_2H$] (*Z* 1). This use of the mass spectrometer as a specific gas chromatographic detector permitted detection at the 10–100 femtomole ($10^{-15}$ mol) level.

The procedure for the quantitative analysis of amino acids as N(O)-perfluorobutyryl-*O*-isoamyl derivatives has been improved (*U8*) and the fragmentation patterns obtained by GC/MS are presented. Horman and Hesford (*U14*) have evaluated *N*(*N'*,*N'*-dimethylaminomethylene)methyl ester derivatives for semiquantitative estimations by direct evaporative techniques. Temperature programming of the ion source permitted construction plots of characteristic masses vs. ion source temperature; the technique is reported to give good results for the traditionally "difficult" amino acids.

The pyrolysis behavior of phenylthiohydantoin derivatives has been described (*U18*) using combined pyrolysis/GC/MS/computer techniques. In addition to mass spectral characterization, the computer-aided analysis of the gas chromatographic pyrolysis patterns is evaluated.

A variety of α-methyl-α-amino acids, which are of interest in extraterrestrial and prebiotic synthesis studies, have been analyzed by gas chromatography and mass spectrometry as the corresponding 2-phenyloxazolin-5-ones (azlactones) (*U9*). These compounds gave relatively simple mass spectra but those of α-propyl-alanine and higher homologues showed no molecular ions. Gas chromatographic and mass spectral data have been compiled for amino acid thiohydantoins and their trimethylsilyl derivatives derived from specific cleavage of the C-terminal amino acid (*U28*).

Interest has continued in the development of mass spectrometric techniques and derivatization procedures for the sequencing of peptides. The EI, CI, and FD spectra of glycylglycine have been recorded using a combined ion source

(*C27*). The utility of field desorption mass spectrometry for sequence studies has been evaluated from spectra of peptides containing three, five, and nine residues (*U1*). The enhancement of volatility is evidenced by the spectrum of the unprotected peptide bradykinin which contains two terminal polar arginine groups; the molecular ion was recorded at *m/e* 1060 together with ions corresponding to a series of overlapping fragments. The addition or removal of hydrogens by surface reactions, and the effects of solvents and inorganic impurities, however, present problems in sequencing unknown peptides. Several FD spectra of peptides have been reported by Rapp et al. (*U29*) and were used to evaluate the products obtained from synthetic procedures.

The problem of differentiation of leucine and isoleucine residues in acetylated/perdeuteriomethylated oligopeptides has been evaluated using unimolecular metastable ion and collision activation spectra (*U17*); the latter spectra gave better structural information as they contained more sequence ions and fewer rearrangement ions, although sensitivity and resolution are comparatively lower.

A rapid heating technique has been described to enhance the volatility of underivatized peptides including those containing arginine (*U2, U3*). Mass spectra were obtained from samples dispersed on Teflon by proton transfer ionization (ionizing reagent $NH_4^+$) and primary fragmentation occurs at the peptide bond together with elimination of small neutral molecules. Spectral correlations permitted determination of the sequence of the arginine-containing nonapeptide bradykinin (*U3*). Mass spectra of arginine and cystine (*C64*) and two tripeptides (*C40*) have been recorded using the new $^{252}Cf$ fission source and a time-of-flight mass spectrometer (see section on Innovative Techniques and Instrumentation).

Schier and Halpern report that trifluoroacetyl/methyl ester derivatives can be synthesized in the tip of a direct insertion probe by pyrolysis of the peptide in the presence of trimethylanilinium hydroxide and methyl trifluoroacetate (*U31*). The pyrolytic methylation procedure was also evaluated for a variety of *N*-protecting groups (*U32*) and the EI spectra gave the molecular and *N*-terminal sequence ions expected for Val-Ile-Ala. The extent of *N*-methylation of the amide groups is discussed and the spectra evaluated for sequence information without purification or isolation of intermediates. The pyrolytic formation of *N*-acetylacetonyl methyl ester derivatives followed by the joint use of electron impact and chemical ionization mass spectrometry provides a direct method for the analysis of dipeptides (*U33*); neither prior separation nor reference compounds are required. The CI spectra gave protonated molecular ion information to complement *N*-terminal residue data from electron impact spectra, and the results were correlated by relative volatility considerations together with corroboration using dimethyltrideuteriomethyl anilinium hydroxide reagent if required.

The isobutane chemical ionization mass spectra of several underivatized peptides have been recorded (*U4*) and evaluated for sequence information. Several of the peptides, however, failed to give any molecular weight information [$(M + 1)^+$ or $(M + 1 - 18)^+$ ions], or sufficient fragment ions to permit residue identifications. The combined use of CI and EI mass spectra permitted an evaluation of the *N,O*-permethylation reaction for peptides prior to sequence studies (*U21*). The various artifacts due to *C*-methylation were found to be dependent on residue position and the structure of neighboring residues.

The development of a peptide-sequencing algorithm for accurate mass measurements is reported by van't Klooster et al. (*U36*). Sequences were constructed from both termini (N → C and C → N) and correct identification relied on self-consistency of the two sequences; the value of elemental compositions was assessed by comparison with the same data after conversion to nominal masses.

Roepstorff and Kristiansen (*U30*) have described the use of a single cycle Edman degradation to eliminate ambiguities in the spectral interpretation of peptide mixtures. The results from the degraded sample were compared with those from the intact peptide and the computed number of possible sequences was shown to be significantly reduced. The alternate use of *p*-chloro- and *p*-bromo-phenylisothiocyanate for the Edman degradation of peptides has been reported to reduce ambiguity in sequence determination by mass spectrometry (*U22*), since the fragment ions of the resulting phenylthiohydantoin derivatives may be easily recognized from their characteristic halogen-isotope pattern.

The value of certain "non-sequence" ions in the spectra of acetylated/permethylated peptides has been reported (*U5*). Two consecutive N–C cleavages with hydrogen rearrangement occur at aspartic acid, asparagine, phenylalanine, histidine, tyrosine, or tryptophan, and are therefore diagnostic of particular residue sequences. A rapid procedure has been proposed (*U6*) for screening sequences in related proteins by comparison with a "template" model.

A related series of peptides containing 2–8 residues and corresponding to the C-terminus of scotophobin has been synthesized and examined mass spectrometrically (*U11*). *N*-Acetylated/*N,O*-permethylated derivatives combined with deuterated analogues ($CH_3CO/CH_3$, $CD_3CO/CH_3$, $CH_3CO/CD_3$, $CD_3CO/CD_3$) were examined to confirm fragmentation pathways and rearrangements.

Several new N-protecting groups have been evaluated by Okada et al. using model peptide methyl esters containing 3 to 12 residues (*U26*). 3-Hydroxyalkanoyl ($C_8$–$C_{18}$) derivatives gave the expected sequence ions together with ions 18 mass units lower because of dehydration to the corresponding 2-alkenoyl derivatives. Both synthesized derivatives gave spectral information at least comparable to acetyl derivatives. The 3-hydroxydecanoyl derivatives were particularly favored as the 18 mass unit doublets made recognition of sequence ions easier.

Pritchard et al. reported the identification of amino acids and dipeptides by derivatization with fluorescamine or 2-methoxy-2,4-diphenyl-3(2*H*)-furanone (*U27*). The spectra show few fragment ions and, for the dipeptides, the base peak corresponds to the ketone of the lactonized derivative; the limited fragmentation behavior may permit sequencing of dipeptides and, as the derivatives fluoresce, they may be easily traced during isolation procedures. Falter et al. (*U7*) have investigated several derivatives which would allow mass spectrometric analysis to be combined directly with established preparative paper chromatography and electrophoresis methods. The nondestructive detection of the peptides was achieved using dansyl chloride, *N,N*-dimethylaminobenzaldehyde, *N,N*-dimethylaminocinnamaldehyde or *N*-hydroxy-succinimido-β-naphthoate, and the resulting derivatives were evaluated from the standpoint of their suitability for mass spectral sequencing. A procedure is described (*U10*) for the removal of Quadrol (used in buffers for automatic protein sequencing) prior to mass spectral residue identification of resulting thiazolinone derivatives of amino acids; boric acid extraction results in the elimination of extraneous peaks in the spectra, permitting more accurate identifications particularly from computer data.

The conversion of oligopeptides to cyclic dipeptides followed by trimethylsilylation has been evaluated by Johnstone and Povall for sequencing by GC/MS (*U15*). Apart from ions (*m/e* 73 and 75) due to the derivatizing function, the spectra gave abundant molecular and (M − 15) ions; however, variable yields of cyclic dipeptides resulted under the conditions used, making the procedure of limited utility at present for small quantities.

The gas chromatographic and mass spectrometric properties have been reported for volatile oligopeptide derivatives formed by reduction of *N*-perfluoroacyl methyl esters with lithium aluminum deuteride (LAD) followed by trimethylsilylation (*U23*). This procedure gives particularly volatile products for all naturally-occuring amino acid residues which permits analysis by GC/MS, and the spectra gave intense sequence ions together with ions corresponding to loss of $CH_3$ from the molecular ion. These derivatives were used in the sequencing of a carboxypeptidase inhibitor isolated from potatoes (*U12*). Accurate mass measurements and the analysis of metastable ions were used to determine the structure of the cyclotetrapeptide Cyl-2, a plant growth inhibitor isolated from a fungus (*U13*).

Recent detailed reports by Kelley et al. (*U16*) and Nau et al. (*U24*) discuss the sequencing of polypeptides by GC/MS analysis of hydrolysis products derivatized as the *O*-trimethylsilylated polyamino-alcohols. The generation of oligopeptide mixtures was optimized with respect to the degree of sequence overlap and a combination of acid hydrolysis and enzymatic digestion was determined to be the most suitable method. The resulting complex mixtures were derivatized and

characterized directly utilizing chromatographic retention indices in addition to mass spectral and mass chromatographic data.

A new technique has been reported for the study of the active sites of enzymes (*U25*). The enzyme is modified by an active-site directed reagent and digested into a mixture of oligopeptides which are derivatized (esterification, acetylation, LAD reduction, trimethylsilylation) and analyzed by GC/MS without further separation or isolation procedures. By comparison with the sequence of the unmodified enzyme, the specific residues of the active site may be determined. The method was exemplified by the identification of Glu-270 in the active site of carboxypeptidase A using a carbodiimide as the enzyme-modifying reagent, and the possible incorporation of $^{18}O$ into the carboxylic groups of Glu-270 or other acidic residues near the active site was also determined.

**Purines and Pyrimidines, Nucleosides, Nucleotides.** The application of mass spectrometry to nucleic acid chemistry has been comprehensively reviewed by McCloskey (*V7*); coverage includes discussion of low and high resolution techniques, the spectra of free and derivatized bases and nucleosides, derivatives of mononucleotides, and sequencing of dinucleotides.

The quantitative detection of purine and pyrimidine bases and nucleosides of pharmacological interest has been undertaken by mass fragmentography with a GC/CIMS combination (*V9*). The $(M + 1)^+$ ions of the permethylated derivatives of model compounds were monitored and permitted detection of arabinosylcytosine at a level of 0.1 mg/ml of serum.

Wilson and McCloskey have undertaken a systematic investigation of the chemical ionization mass spectra of nucleosides using a variety of reagent gases (*V14*). As well as protonated molecular species, the spectra show a principal ion corresponding to the (base + 2 H) arising from initial base protonation hydrogen transfer from O–2′ and cleavage of the glycosidic bond. Estimated proton affinities provided a relative basicity scale for the common bases and nucleosides; in the gas phase, nucleosides were found to be more basic than their corresponding purines or pyrimidines. CI and EI spectra were recorded for several purines and pyrimidines derivatized by an improved method for *N*-methylation (*V1*).

The differentiation of 3′- and 5′-*O*-substituted nucleosides has been achieved by a GC/MS method (*V11*). The *tert*-butyl-dimethylsilyl derivatives are separable by gas chromatography, are less easily hydrolyzed compared to TMS or TFA derivatives, and give characteristically different spectra for the 3′- and 5′-isomers of thymidine and deoxyadenosine.

Further studies are reported on the mass spectra of pyrolysis products of nucleic acids (*V10*). Using the Curie-point pyrolysis technique, spectra of DNA and RNA were recorded by both low voltage ionization and high resolution field ionization for comparison; the accurate mass measurements confirmed that the carbohydrate moiety produced the majority of the resulting ions, and key fragments permitted differentiation of DNA and RNA at the microgram level.

Liehr et al. (*V5*) have examined the origin of the [base + 41] ion that is characteristic in electron impact spectra of cytosine nucleosides. Using low and high resolution spectra together with TMS, TFA, and permethylated derivatives and labeling techniques, a mechanism for the transfer of $C_2HO$ from the sugar to the base was proposed. The electron impact induced elimination of methylenimine is important in the structural characterization of several methylated purine bases or nucleosides and the mechanism of this reaction has been studied in dimethylamino nitrogen-heterocycles using deuterium-labeled model compounds (*V13*). Mass spectra obtained of gas chromatographic effluents were used to determine the extent of trimethylsilylation of nucleosides synthesized for a gas chromatographic study (*V3*). McCloskey et al. have discussed the mass spectral characteristics of trimethylsilyl derivatives of *N*-succinyl metabolites of adenine and aminoimidazole carboxamide, and $N^6$-(2-succinyl)-adenine was identified in human urine by liquid chromatographic fractionation followed by GC/MS (*V8*).

Direct insertion low resolution mass spectrometry was used to analyze the products obtained from treatment of synthetic polynucleotides with the antitumour agent 1,3-bis(2-chloroethyl)-1-nitrosourea, which is known to possess alkylating activity and which may modify cellular DNA and RNA. After incubation, nucleotides were obtained by chemical or enzymatic methods and were analyzed as their corresponding nucleoside trimethylsilyl derivatives (*V6*) A similar procedure using GC/MS together with liquid and thin layer chromatographic techniques was used to sequence the 5′-terminal oligonucleotide from U-2 ribonucleic acid (*V12*).

Kempster et al. (*V4*) have reported field ionization mass spectra of free bases derived from $HF/BF_3$ hydrolysis of nucleic acids, and two fluorescent compounds derived from $N^6$-($\Delta^2$-isopentenyl)-adenosine have been characterized (*V2*).

## CARBOHYDRATES

Lönngren and Svensson have published a detailed review on the structural analysis of natural carbohydrates by mass spectrometry (*W14*). The scope includes monosaccharides derivatized by permethylation, peracetylation, trimethylsilylation, and partial methylation; monosaccharide alditol acetates, trifluoroacetates, methyl ethers, trimethylsilyl ethers, and partially methylated alditol acetates; various additional monosaccharide derivatives; and derivatized oligosaccharides.

The field desorption mass spectra of D-glucurono-6,3-lactone, L-gulono-1,4-lactone, xylitol and L-sorbose have been recorded (*W3*); the spectra show a single (M + 1) peak at low emitter temperatures and this ionization technique is considered to be a useful addition to current methods (see section on Field Ionization and Field Desorption). Dougherty et al. have studied the CI mass spectra of oligosaccharide peracetates using a 2:1 mixture of ammonia and isobutane as the reagent gas (*P8*); the spectra of the di-, tri-, and tetra-saccharide derivatives showed intense ions corresponding to an $(M + NH_4)$ ion, and individual monosaccharides could be determined from similar ammonium ion complexes with thermolytically-derived neutral fragments. Horton et al. (*W10*) have assessed the utility of chemical ionization techniques for sugar derivatives with both isobutane and ammonia as reagent gases (see section on Chemical Ionization); the spectra are particularly simple and generally give molecular ion information from $(M + H)$ or $(M + NH_4)$ ions. The limited fragmentation results from simple dehydration or cleavage of substituent groups. A detailed study of fragmentation of 1,6-anhydro-3,4,*O*-isopropylidene-β-D-talopyranose has been undertaken by Horton et al. using high resolution electron impact spectra of specifically deuterated derivatives (*W9*); a comparison of the chemical ionization spectra with ammonia and isobutane reagent gases was also reported. The fragmentation of methyl (methyl 2,3,4-tri-*O*-methyl-α-D-glucopyranosid)uronate at 70 and 12 eV electron energies has been studied using various trideuteriomethyl derivatives (*W11*); the low energy spectra contain only the primary fragments and are therefore easier to interpret, and are preferred for structure elucidation of monosaccharide methyl ethers. The related amine has been similarly investigated (*W12*) at low and high ionizing energies incorporating $CD_3$- and $ND_2$-labeled groups; a new fragmentation series results from the presence of the amide function. Specifically deuterated derivatives and high resolution mass measurements were used to determine the fragmentation behaviour of *N*-acyl derivatives of daunosamine, the glycoside moiety of certain antitumour antibiotics (*W27*), and a facile stereospecific elimination of MeOH was found to occur for methyl β-daunosaminides.

Studies have continued on the mass spectra of derivatives which are suitable for analysis by GC/MS. Pertrimethylsilylation is particularly popular and reports include TMS derivatization of alditols and acids derived from alkaline degradation of partially methylated glucoses and galactoses (*W1*), deuterated alditols from reduction of aldoses, ketoses and lactones (*W5*), *O*-methyloximes of 2-acetamido-2-deoxyaldoses (*W20*), branched deoxyaldaric acids from 4-*O*-substituted uronic and ulosonic acids (*W21*), partially methylated sugars (*W15*), glucuronic acids (*W16*), and benzene-, butane-, and methane-boronates of pentoses, hexoses, and acetamido-hexoses (*W22*). Other studies by GC/MS include identification of aldonic and uronic acids as deuterium-labeled alditol acetates (*W24*), per-*O*-acetylaldono-nitriles (*W25*) and *O*-isopropylidene aldose derivatives (*W19*), methyl ethers of 2-deoxy-2-(*N*-methylacetamido)-D-glucose (*W23*), and partially methylated *N*-methylglucosamines (*W26*).

Wood and Siddiqui have reported the spectra of boronic esters of xylose, arabinose, fucose, glucose, fructose, and glyceraldehyde (*W28, W29*); butane boronates, silylated if

necessary, are preferred for gas chromatographic analyses, but benzene boronates may be more suitable for some applications because of their crystallinity. The condensation of saccharides with substituted hydrazones has been investigated with the view to mass spectrometric analysis (*W13*). Without derivatization, hydrazones of pentoses and hexoses are thermally destroyed but satisfactory spectra could be obtained from peracetates of monosaccharide hydrazones and are discussed.

The diagnostic value of mass spectra of carbohydrate enones has been evaluated by Holder and Fraser-Reid (*W8*) using confirmatory accurate mass measurements on selected ions. Two main fragmentations were observed: the direct loss of ring substituents, and the *retro*-Diels–Alder type cleavage. The latter process permits location of the position of the $\alpha,\beta$-unsaturated keto chromophore in these molecules. High resolution measurements were also used in a study of the reaction products obtained from sugars containing vicinal cis- or trans-amino-alcohol groups on treatment with benzeneboronic anhydride (*W17*).

The sequence analysis of small oligosaccharides has received further attention. Guerrera and Weill (*W7*) have discussed the competing primary fragmentations of maltose acetate including some iodo derivatives, and the permethyl and pertrimethylsilyl derivatives of lacto-*N*-tetraose have been evaluated for mass spectral sequence information (*W6*). Colard et al. (*W4*) have determined the sequence of the trisaccharide portion of a new saponoside, and spectra are reported for the permethylated saponoside and its methanolysis products, as well as for various alditol derivatives obtained by reduction with $NaBH_4$ and $NaBD_4$. The permethyl ethers of 25 oligosaccharides have been studied by Moor and Waight (*W18*); reproducible spectra could be obtained by careful purification of the parent sugar prior to methylation. The fragmentations gave structural information on the presence of fructose units, the pyranose/furanose ratio and the position of the glycosidic linkage, and thus preference is given to methylated derivatives compared to trimethylsilyl ethers for structure determination.

Partial hydrolysis and GC/MS of the resulting oligosaccharides as alditol acetates was used to study the sequence of the capsular polysaccharide from *Klebsiella* Type 52 (*W2*) but anomeric residues could not be differentiated.

**Complex Lipids.** This section summarizes the main developments related to complex glycosides (glycolipids), phosphorus-containing lipids (including sphingolipids), and complex lipids which contain sphingosines (ceramides and cerebrosides or sphingoglycolipids).

A review of the literature prior to 1974 has appeared (*X37*) on the GC/MS analysis of large polar lipids. Coverage includes sample preparation and instrumentation, separation and characterization studies, and applications to glycerophospholipids, sphingosines, ceramides, sphingophospholipids, sphingophosphonolipids, and sphingoglycolipids.

The high resolution field desorption mass spectra of a variety of underivatized glycosides have been recorded (*X33*) and the identification of the sugar and aglycone moieties can be deduced from the observed fragmentation patterns. This ionization technique provides molecular weight information which is difficult to obtain from electron impact spectra of unmodified compounds, but the presence of ions such as $[M + {}^{23}Na]^+$ and $[M + {}^{39}K]^+$ attributed to Na and K salt impurities would make the determination of molecular weights of unknown compounds ambiguous.

Electron impact studies have been reported for the structure determination of a variety of synthetic and biologically-derived glycosides. Batrakov et al. (*X1, X2* and references therein) have discussed the fragmentation behavior of derivatized monoglycosyldiglycerides and summarize the structural information that can be derived. Natural derivatives of neuraminic acid have been investigated by Kammerling et al. (*X14, X15*) utilizing both high and low resolution measurements. Trimethylsilylated methyl esters gave characteristic spectra permitting identification of *N*- and *O*-acyl groups, and differentiation of $(2 \rightarrow 3)^-$ and $(2 \rightarrow 6)$-linked isomers of *N*-acetylneuraminic acid-lactose. GC/MS was used to identify acetylated diglycerides derived from phosphatidylcholine (*X12*) after TLC separation according to the degree of unsaturation of the long-chain acyl groups; mass spectral data gave the structure and location of the fatty acid residues attached to glycerol. Examples of other uses of mass spectral data to identify glycosides may be found in the following papers: *X4, X8, X24, X31, X38* Specific mention should be made of a study of steroid saponins by high resolution mass spectrometry involving accurate mass measurements by photoplate detection of high mass ions exceeding *m/e* 1000 (*X25*).

Phospholipids are generally analyzed by mass spectrometry after degradation (removal of phosphate ester or fatty acids) and subsequent derivatization (see, e.g., *X3, X21, X22*). This approach has been utilized by Curstedt and Sjövall (*X7*) to study the incorporation of deuterium derived from metabolized [1,1-$^2H_2$]-ethanol into phosphatidylcholines isolated from rat bile. Most of the deuterium was found to be located in the glycerol portion, and time-dependent measurements following ethanol administration may be related to the metabolic turnover rate of phosphatidylcholine. Einolf and Fenselau (*X9*) describe the identification of trimethylsilyl derivatives of $\alpha$-glycerophosphoryl-glycerol and -inisitol as moieties of phospholipids derived from human alveolar secretion. Karlander et al. (*X16*) report a selective *N*-demethylation procedure to allow GC/MS analysis of the polar phosphate and phosphonate moieties of choline-containing lipids. A similar procedure formed part of the methods used in detailed structure determinations of sphingomyelins (ceramide phosphorylcholines) and ceramides isolated from bovine kidney (*X23*).

Preliminary studies on the analysis of intact phospholipids by field desorption mass spectrometry have been reported (*X10, X40*); molecular weight information may be derived from molecular or "quasimolecular" (M + 1) ions and structurally-significant fragments have been identified, indicating the potential utility to the study of natural mixtures.

The characterization of sphingolipids by mass spectrometry has continued to attract attention. Markey and Wenger (*X29*) have compared electron impact and chemical ionization spectra of acetylated and perdeuterio-acetylated derivatives of ceramides, cerebrosides, and ceramide dihexosides, and also include an evaluation of the problems involved in the analysis of such polar, polyfunctional molecules by electron impact ionization. The chemical ionization spectra, obtained using methane as the reagent gas, show abundant high mass ions corresponding to protonated molecular ions or to the loss of $H_2O$, $CH_3OH$ or $CH_3CO_2H$ from the (M + H) ion. Maximum structural information may be derived from the combined use of both techniques. The detection of cerebroside molecular ions in electron impact spectra has been reported by Ohnishi (*X30*); a mixture of trimethylsilyl derivatives was introduced via a glass chromatographic column and glass interface, and molecular ions (deduced from lower mass ions) were detected at *m/e* 1259, 1257, 1171, and 1169 in the spectrum obtained from the major chromatographic peak.

A detailed study on the fragmentation behavior of bis(*O*-trimethylsilyl-*N*-acetyl)sphinganine has appeared (*X27*) and utilizes low resolution GC/MS, accurate mass measurement and perdeuterio-trimethylsilylation techniques. The mass spectra of a series of glycosphingolipids using permethylated derivatives have been evaluated for structural studies (*X28*).

Other studies include glycosylceramides isolated from human erythrocyte membrane (*X11, X36, X39*), ceramides from rabbit leukocytes (*X6*), long-chain bases of sphingophosphonolipids from *Turbo cornutus* (*X13*), glycosphingolipids from the salt gland of spiny dogfish (*X22*), and cerebrosides from a marine sponge (*X32*).

A series of papers has appeared by Karlsson and co-workers on the mass spectral characterization of glycosylceramides isolated from various tissues including bovine and dog digestive tracts, horse kidney, bovine brain, and human tumors and small intestine (*X5, X18–20, X34, X35*). Of particular note is the identification of derivatives of hexaglycosylceramide of brain tissue (*X17*) which involved measurement of molecular weight ions at *m/e* 2245. This was achieved on about 10 mg of material using an AEI MS-902 mass spectrometer operated at 30 eV and 3.2 kV accelerating voltage. The authors point out that "... this glycolipid is the largest organic molecule so far analyzed in the gas phase with structural information on the complete molecule".

**Prostaglandins.** Gas chromatography/mass spectrometry has continued to be an important technique for the identification and quantitation of prostaglandins and their metabolites. However, as summarized by Samuelsson et al. in a gen-

eral review (*Y25*), care should be taken in the interpretation of data on endogenous levels of prostaglandins because of increased or continued biosynthesis during sample handling, production by autoxidative cyclization, and release from platelets during collection and handling of plasma and serum.

A review of mass spectrometry of prostaglandins has been published by Crain et al. (*Y2*) and includes a guide to published spectra, preparation of derivatives, spectral interpretation and quantitative determination using deuterium-labeled internal standards and multiple ion monitoring of gas chromatographic effluents.

Several papers have appeared on the use of chemical ionization techniques in GC/MS analyses (see Chemical Ionization section). Oswald et al. (*Y24*) evaluated the electron impact and CI spectra using both methane and isobutane as reagent gases for underivatized $PGE_2$ and $PGF_{1\alpha}$, and for trimethylsilyl, acetyl, and trifluoroacetyl derivatives of prostaglandin methyl esters. GC/CIMS using both methane and helium reagent gases was used to identify prostaglandin products formed from the incubation of adrenic acid with sheep vesicular gland microsomes (*Y32*). Following purification by thin layer chromatography, 1a,1b-dihomo-$PFG_{2\alpha}$ was identified as the methyl ester/TMS ether, and 1a,1b-dihomo-$PGE_2$ was identified as the methyl ester/methoxime/TMS ether; both types of CI mass spectra are shown for these homologues and for the corresponding derivatives of $PGF_{2\alpha}$ and $PGE_2$.

Elucidation of the characteristics of electron impact mass spectra of prostaglandins has continued to receive attention. Middleditch and Desiderio studied the alkyloxime/TMS ester/TMS ethers of prostaglandins $A_1$, $B_1$, $E_1$, and $F_{1\alpha}$ utilizing high resolution MS data and $d_9$-TMS labeling (*Y20*); certain fragmentation processes were found to be common to all spectra and others were unique to the particular prostaglandin under study. The mass spectral behavior of prostaglandin $A_1$ and its methyl ester (*Y17*) and the methyl esters of $E_1$ and $E_2$ (*Y16*) have been reported; low electron voltage spectra, metastable ion decomposition studies, high resolution MS data and deuterium labeling were used to elucidate fragmentation mechanisms.

Watson and Sweetman (*Y33*) have compared the spectra of various derivatives of $PGA_1$, $PGA_2$, $PGB_1$, and $PGB_2$ in order to evaluate their usefulness for quantitative analysis by multiple ion monitoring of gas chromatographic effluents; the derivatives studied were the methyl ester/TMS ether, TMS ester/TMS ether, and methyl esters additionally derivatized as *tert*-butyl-dimethylsilyl ether, methoxime/TMS ether, acetate, and methoxime/acetate. The spectra permitted differentiation between the PGA and PGB isomers, particularly in the case of methyl ester/silyl ethers and persilylated derivatives.

The use of *N*-trimethylsilylimidazole in the presence of piperidine has been reported for the rapid quantitative derivatization of prostaglandin methyl esters to give single products with suitable gas chromatographic properties (*Y22*); quantitation of these derivatives of standard $PGF_{2\alpha}$ and $PGE_2$ by GC/MS with multiple ion monitoring was found to be linear over the range 2.5 to 170 pmol using tetradeuterated analogues as internal standards. The method has been used to study the biosynthesis of these prostaglandins in slices of rat cerebral cortex during incubation in the absence of added precursors (*Y21*, *Y23*).

The quantitative analysis of prostaglandins by mass spectrometric methods has been summarized recently by Green et al. (*Y10*). Quantitation may be accomplished by multiple ion monitoring using a deuterium-labeled analogue, or by using an unlabeled homologue as internal standard and monitoring a single common ion. Following the method proposed by Lee and Millard (*Y19*), Cory et al. have reported a standard deviation of 8.5% for 5 determinations of 10 pg of prostaglandin $F_{2\alpha}$ methyl ester/TMS ether using single ion monitoring of *m/e* 423 (*Y1*); a tetradeuterated analogue was used as the carrier and an unlabeled homologue acted as the internal standard for quantitation.

The GC/MS technique with selected ion monitoring is now being used in a variety of biochemical studies on prostaglandins. Frolich et al. have measured $PGA_2$ levels in human plasma from normal subjects before and after dietary sodium depletion in an investigation of the possible role of this prostaglandin as a circulating hormone (*Y5*, *Y6*). $PGE_2$ and $PGF_{2\alpha}$ have been detected and quantitated by mass spectrometry in human female urine at levels of 374 ± 77 pg/ml and 386 ± 78 pg/ml respectively, and additional studies indicate their origin from intrarenal synthesis (*Y7*). The same prostaglandins have been identified in the incubation medium of whole-cell preparations of rat renal papilla (*Y3*) in a study of the stimulatory effect of angiotensin II on renal prostaglandin biosynthesis.

The association between increased prostaglandin production and hypercalcemia in neoplastic disease states has been described by Seyberth et al. (*Y27*) by measuring the urinary excretion of 7α-hydroxy-5,11-diketotetranorprostane-1,16-dioicacid—themajorurinarymetaboliteof$PGE_1$and$PGE_2$—as an index of prostaglandin biosynthesis. Samuelsson and Green also measured prostaglandin metabolites as a means for monitoring $E_2$ and $F_2$ synthesis in humans (*Y26*); unlike the parent compounds, the 15-keto-13,14-dihydro-metabolites have not been reported to be formed in blood and thus permit analyses to be carried out on peripheral plasma. Levels of ~50 pg/ml and ~25 pg/ml were determined for the $F_2$ metabolite in male and female plasma respectively, and ~28 and ~21 pg/ml were measured for the $E_2$ metabolite.

The relationship between endogenous prostaglandin synthesis and human pregnancy and parturition has been investigated by mass spectrometric quantitation of the major urinary metabolite of $PGF_1$ and $PFG_2$—5α,7α-dihydroxy-11-keto-tetranorprostane-1,16-dioic acid (*Y11*), and of plasma levels of the 15-keto-13,14-dihydro-metabolite of $PGF_{2\alpha}$ (*Y8*). The latter metabolite and the parent prostaglandin have also been quantitated in biopsies of human endometrium before and after IUD insertion (*Y9*), and $PGF_{2\alpha}$ and $PGE_2$ have been quantitated in human endometrium during the normal menstrual cycle (*Y4*).

A series of publications has appeared utilizing mass spectrometric methods for structure identification and/or quantitation of prostaglandin endoperoxides (*Y12–15*, *Y29*); the endoperoxides and related metabolites were formed from incubations of arachidonic acid and are implicated in the mode of action of prostaglandins on platelet aggregation.

Further studies have been reported on the identification of prostaglandins in human seminal fluid using GC/MS techniques. The 19-hydroxy analogues of $PGE_1$ and $PGE_2$ have been reported by Taylor and Kelly (*Y31*) and by Jonsson et al. (*Y18*), and occur in significantly larger quantities than the corresponding analogues of A and B series; the presence of 19-hydroxy-$F_{2\alpha}$ and -$F_{1\alpha}$ has also been demonstrated (*Y30*) together with indications of isomeric analogues. GC/MS analyses were used to identify derivatives of a variety of urinary metabolites obtained from chronic intravenous infusion of tritium-labeled $PGF_{2\alpha}$ in rats (*Y28*).

**Biomedicine and Clinical Chemistry.** Mass spectrometry has continued its expansion in the field of the biomedical sciences, although it is still not routinely used in clinical laboratories. In research environments, the general approach encompasses studies of normal human biochemistry undertaken in parallel with studies of disease states, and is followed here.

Interest in GC/MS techniques is evidenced by the 1973 Montreal Workshop on the application of GC/MS to the investigation of human disease (*Z52*), a one-day conference on GC/MS in laboratory medicine sponsored by the National Institute of General Medical Sciences (*Z56*), and a symposium on the identification of metabolites using GC/MS (*Z15*).

Mass spectral data of compounds of endogenous physiological origin have been compiled by Markey, Urban, and Levine in collaboration with Committee VI of the American Society for Mass Spectrometry (*Z54*). Volume 1 contains an alphabetical index of compound names, an index for the most intense peak in each 14 mass units between *m/e* 15 and 168 for compounds with molecular weights <168, and an index for the most intense peak in each 50 mass units between *m/e* 100 to 650 for compounds with molecular weights >168. Volume 2 (parts 1 and 2) contains plotted spectra and tabular listings in order of molecular weight, together with operational parameters when known. The spectra are available in Aldermaston "D" format on magnetic tape.

Lawson (*Z44*) has reviewed the scope of mass spectrometry in clinical chemistry and covers methodology and instrumentation, structure identifications of physiological compounds (biogenic amines, thyroid hormones, amino acids,

peptides, carbohydrates, lipids, prostaglandins, steroids), inborn errors of metabolism, and clinical applications (volatiles in body fluids, respiration and blood gases, stable isotopes, clinical toxicology, and drug studies).

The principles and techniques of mass spectrometry, together with spectral interpretation, have been summarized by Völlmin (*Z83*) with reference to biomedical compounds, and the paper contains several spectra of representative compound classes. Eldjarn et al. (*Z29*) have summarized the clinical applications of GC/MS encountered by the Oslo group, and the approach which has developed as the result of nearly a decade's use of the technique for the study of metabolic disorders. A more recent development is the automatic recognition of anomalous components in complex mixtures (*Z37*). Although applicable in theory to any complex mixture, the computer search has been evaluated in terms of identifying abnormal and potentially pathological metabolic profiles—either the presence of an abnormal component or the absence of a "normal" metabolite—by comparison with a "normal" reference sample run under nominally identical conditions. The program utilizes some measure of chromatographic retention time (using a spectrum number window) but makes no attempt to structurally identify the anomalous spectrum. With refinements, this approach should permit faster evaluation of metabolic profiles obtained from screening of physiological fluids.

The problem of rapid structure identification of components in mixtures of biological origin has been addressed by Sweeley et al. (*Z81*) by criteria involving a gas chromatographic retention index (*X70*) in conjunction with a limited but highly specific set of "discriminating" ions. A library file is compiled for each compound consisting of a retention index (which will be dependent on the liquid phase used), a primary differentiating ion, and a set of "confirming" ions; the selected ions are chosen not just to be characteristic of the compound but also to attain maximum differentiation from other compounds having similar chromatographic properties. The system has been evaluated using urinary acidic metabolites, and the factors affecting the accuracy of peak identification are discussed.

The utility of GC/HRMS, providing accurate mass measurements of all peaks in spectra obtained by repetitive scanning, has been assessed for the analysis of urinary organic acids (*Z41a*) and the use of specific elemental composition (accurate mass) chromatograms is illustrated (*Z41b*).

Lee and Millard (*Z47*) have undertaken an evaluation of unlabeled vs. labeled internal standards for quantitative studies by single and multiple ion monitoring. For the determination of methylated allobarbitone, they concluded that the most accurate and sensitive method involves the use of a labeled analogue as a carrier, together with an unlabeled standard which gives an ion in common with the compound being measured, thus permitting single ion monitoring.

Mass spectra obtained by electron impact, chemical and field ionization, and field desorption techniques have been compared for a variety of biologically important compounds (*Z31*); spectra are presented for amino acids (leucine, isoleucine, norleucine, creatine), steroids (tetraol and diol-dione of cholest-5-ene), triglycerides (tricaproin, trilaurin), drugs (talbutal, phenobarbital, mephobarbital, ephedrine), and pesticides (phosphamidon, temik, delnar) and are evaluated in terms of structure identification. It is important to note that for FI, FD, and CI where there may be very few ions in the spectrum, there is a particular problem with the identification of the molecular weights of unknown samples, since high mass ions may represent M or (M + H), or in CI spectra M, (M − H) or (M + R). The availability of all techniques is recommended for specific usage depending on the particular problem (see subsections on FI, FD, and CI Techniques in Ion Chemistry section).

The chemical ionization technique has also been reported for quaternary amines related to the neurotransmitter acetylcholine, and for ethidium bromide and its acetylated derivatives (mutagenic intercalating dyes); major ions in the spectra—obtained using isobutane as the reactant gas—corresponded to known thermal decomposition products of these amines. The use of reagent gases ($N_2$, Ar, and He) containing 2–15 mol % nitric oxide has been evaluated for the determination of trimethylsilyl derivatives of biologically important compounds by chemical ionization (*Z38*). The spectra show enhanced intensity of molecular ions together with retention of the major fragment ions and some loss of intensity for low mass ions of limited structural value.

The identification of metabolites in human body fluids has particular clinical relevance to the study of inherited metabolic disorders such as those associated with amino acid metabolism (*Z72*, *Z74*), and the role of clinical chemistry in the diagnosis of these problems has been discussed by Eldjarn et al. (*Z30*) and Chalmers and Lawson (*Z18*).

Many metabolic disorders are characterized by abnormalities in the urinary profiles of organic acids and further refinements in the analysis of these metabolites have been made. Various isolation methods for urinary acids have been evaluated in detail (*Z82*); anion exchange extraction with DEAE Sephadex proved to be more efficient and precise when compared with continuous solvent and manual solvent extractions, a prerequisite for the quantitative study of metabolite levels in disease states. A methylation procedure has been described which prolongs stability of aromatic acid derivatives in solution during storage (*Z33*); the method involves conversion of the acids to their trimethylanilinium salts, and pyrolysis in the GC injection port generates methylated derivatives for GC/MS identification.

The analysis of α-ketoacids as pertrimethylsilyl derivatives is difficult because of the formation of multiple components and limited structure information in their mass spectra; Lawson et al. (*Z45*) have further studied the methyl-, ethyl-, and benzyl-oxime/trimethylsilyl ester derivatives for GC/MS analysis of these acids, and their mass spectra are discussed. The ethoxime/TMS derivatives have been used to quantitate a variety of urinary metabolites in studies of patients with β-methylcrotonylglycinuria, propionic acidemia, and methylmalonic aciduria (*Z17*), and in samples from 1778 mentally-retarded patients and 420 controls (*Z87*). Similar investigations on the urinary excretion of unconjugated aromatic acids by phenylketonuric patients have been reported (*Z19*).

The value of high resolution glass capillary columns has again been emphasized (*Z42*) and little qualitative variations were found for the urinary acid profiles from control and postpartum subjects. GC/MS has also been used to study the urinary excretion of *n*-hexanedioic and *n*-octanedioic acids in patients with untreated juvenile diabetes mellitus (*Z73*). Elevated levels of these acids in patients with ketonuria could be normalized by insulin therapy, whereas the excretion of 3-methylhexanedioic acid (which is probably derived from branched fatty acids produced by intestinal microflora) was unaffected by the treatment.

α-Methylacetoacetic, α-methyl-β-hydroxybutyric, acetoacetic, and β-hydroxybutyric acids as well as tiglylglycine have been identified in urine from a patient with ketoacidosis (*Z35*); the analysis permitted further detailed clinical studies to be undertaken and a primary enzyme defect in isoleucine degradation was suspected.

GC/MS and high resolution mass measurements have been used to provide a conclusive method to identify *m*-hydroxyphenylhydracrylic acid in urinary extracts as the methyl ester or bis(trimethylsilyl)ether/methyl ester (*Z27*). The level of excretion of this acid has been noted to be highly variable and its recognition is therefore important in metabolic screening processes.

Mass spectrometry provided confirmatory data in the gas chromatographic resolution of enantiomers of methylsuccinic acid isolated from human urine (*Z89*); the acid was derivatized as the S-(+)-2-butyl ester following TLC separation, and was identified as the R-(+)-isomer by comparison with an authentic sample. The enantiomeric composition of β-aminoisobutyric acid in human serum and urine has been determined by formation of *N*-TFA/S-prolyl-dipeptides (*Z80*), and quantitated as the *N*-TFA/*n*-butyl ester. Urine samples contained the R-isomer (probably derived from the degradation of thymine), whereas serum samples contained predominantly the S-isomer (80%) of unknown origin.

The presence of 2-ethylhydracrylic acid in normal human urine and its elevated excretion after oral isoleucine administration has prompted a mass spectral study of the deuterated acid and other metabolites excreted by rats following intraperitoneal injection of deuterated 2-methylbutyric acid (*Z53*); the results provide evidence for an alternate minor catabolic pathway for isoleucine.

Further studies on the volatile components of human urine

by GC/MS techniques have been reported for normal individuals and for patients with diabetes mellitus (*Z50*). Abnormally high levels of low molecular weight alcohols and ketones were determined to be related to the metabolic disorders in diabetic patients (*Z49*), and mass chromatography was used for more specific detection of these compounds (*Z48*).

Zlatkis et al. (*Z90*) have described a method for the analysis of volatile metabolites in human serum and plasma utilizing GC/MS for structure identification, and the volatiles in pooled normal blood plasma and of plasma obtained before and after hemodialysis have been studied (*Z26*). The mass spectral measurement of gas tensions in blood and respiratory studies concerning lung physiology have been reviewed (*Z43*).

Mrochek and Rainey (*Z64*) have described the use of GC and MS for the identification of trimethylsilyl derivatives of glucuronides isolated from human urine by high resolution liquid chromatography. The mass spectra obtained are evaluated in terms of identification of glucuronide conjugation and the nature of the aglycon.

Oligosaccharides containing mannose have also been characterized in the urine of patients with mannosidosis (a lysosomal storage disease) by GC and GC/MS methods (*Z71*); one trisaccharide was identified as α-D-mannopyranoside-(1 → 3)-β-D-mannopyranoside-(1 → 4)-2-acetamido-2-deoxy-D-glucose by mass spectral interpretation of the permethylated alditol derivative and comparison with an authentic sample (*Z51*). This component was present in all mannosidosis urines (123–469 mg/L as quantitated by GC), but was not detected in normals or heterozygotes, allowing confirmation of enzymatic diagnosis of mannosidosis.

GC/MS methods for the analysis of steroids have continued to be investigated (see, e.g., *Z8*, *Z9*, *Z46*, *Z55*, *Z79*, *Z84*). Chemical ionization mass spectra have been reported for steroidal ketones (*Z57*) and sterol esters (*Z65*), and field desorption mass spectrometry was used in the analysis of estriol-16α-glucuronide isolated from pregnancy urine (*Z3*). Adlercreutz et al. have described a mass chromatographic method for steroid determinations in various biological fluids (*Z2*) and quantitatively determined 11 estrogens in body fluids of pregnant and nonpregnant subjects (*Z4*). Fractionation of pregnancy urinary steroids using Sephadex LH-20 has been described prior to GC/MS investigations (*Z10*) and the quantitation of estriol in human pregnancy urine using a deuterated analogue as internal standard is reported (*Z13*). The quantitative measurement of urinary tetrahydroaldosterone has been described (*Z75*), and androstenetriolones and androstenetetrols have been characterized in the urine of infants by GC/MS (*Z76*).

GC/MS analyses are also reported for determinations of serum cholesterol (*Z12*), unconjugated neutral steroids in plasma (*Z6*) and tissues (*Z5*), and plasma cortisol (*Z11*), testosterone, progesterone, and androstenedione (*Z23*). The quantitative determination of testosterone levels in human male plasma is being evaluated for measurements of the lower levels present in female plasma, and direct sample introduction and mass chromatographic monitoring at a resolution of 3000 is discussed for samples isolated by thin layer chromatography (*Z20*).

Millington has described the measurement of endogenous steroids in biological extracts by monitoring a selected single ion at high resolution (8 500–10 000) in gas chromatographic effluents (*Z58*); the method has been used in studies of steroid concentrations in human breast tumors (*Z60*) and hyperplastic prostate tissues (*Z59*).

Other studies have been reported on GC/MS identifications of aromatized steroids produced by human placental microsomes (*Z14*), plasma bile acids in pregnant women with intrahepatic cholestasis (*Z7*), and bile acids and cholesterol in bile (*Z62*).

The mass spectral identification of biogenic amines and their metabolites has continued to receive attention and reports have appeared on the use of dansyl (*Z28*), TMS (*Z1*), *N*-TFA/*O*-TMS (*Z25*), and *O*-ethyl ether (*Z66*) derivatives. Chemical ionization mass spectrometry of gas chromatographic effluents has been utilized for analyses of choline and its esters (*Z36*) and of a variety of amines and their metabolites found in cerebrospinal fluid (*Z61*). Several publications have appeared on GC/MS studies of metabolites in normal human physiological fluids (*Z40*, *Z67*, *Z77*, *Z78*, *Z88*) and in samples from Parkinson patients (*Z68*, *Z69*), schizophrenics (*Z21*, *Z32*), and subjects with hyperthyroidism, hypertension, neuroblastoma, and pheochromocytoma (*Z85*, *Z86*).

The determination of amino-acetone and S-amino-levulinic acid in human serum and urine by GC and GC/MS has been described (*Z34*); the quantitation of these aminoketones in body fluids, utilizing trimethylsilylated pyrrole derivatives is of diagnostic importance in cases of lead intoxication and acute intermittent porphyria. The mass spectral identfication of indole-3-carboxylic acid in the urine of normal and pathological subjects is also reported (*Z16*).

A low voltage (20 eV) mass chromatographic analysis of tryptophan metabolites in human cerebrospinal fluid has been described (*Z22*) using the pentafluoropropionyl derivatives. 5-Hydroxytryptophol and 5-methoxytryptophol were identified at concentration levels of 0.1–33 ng/ml and 0.3–13.9 ng/ml, respectively; the considerably higher levels of 5-hydroxyindoleacetic acid in CSF indicate that reductive metabolism of cerebral 5-hydroxytryptamine to tryptophols is a relatively minor pathway. A GC/MS method was used to identify dipeptides isolated from the urine of a patient suffering from dermatological purpura, the results indicating the possibility of a collagen abnormality (*Z39*).

The determination of urinary $^{15}N/^{14}N$ by mass spectrometry has been used to study the retention of nitrogen in growth hormone deficient children (*Z24*); the patients were administered $^{15}N$-labeled glycine and treatments with human growth hormone and androgen (oxandrolone) were evaluated. The fragmentation patterns of biologically important porphyrins isolated from urine and feces from porphyric humans have been discussed (*Z63*).

**Pharmacology.** The use of mass spectrometry in the field of drug metabolism has been recently reviewed by Millard (*B16*, p 339); coverage includes low resolution studies on reference compounds and metabolites, quantitative GC/MS and high resolution and chemical ionization mass spectrometry. Mass spectrometric techniques have been used to identify the metabolites of a variety of drugs administered to human subjects or patients. GC/MS with specific ion monitoring is the popular approach to obtain the sensitivity essential in analyses of biological fluids, and the use of deuterated analogues appears to be almost routine for quantitative work. GC/MS techniques have been reviewed by Fenselau (*D19*), with examples of pharmacological and toxicological applications and the use of stable isotope analyses.

Several reports have appeared on the use of chemical ionization mass spectrometry (see CI portion of Ion Chemistry section) for drug studies in humans. Using the direct insertion inlet and with isobutane as the reagent gas, quantitative plasma determinations using deuterium-labeled analogues were reported for the anti-arrhythmic agents quinidine and lidocaine administered to patients and volunteers (*AA31*); between 5 ng and 4 μg of lidocaine could be detected by this method, and time course profiles were measured for the two drugs as well as for dihydroquinidine (present in commercial sources of quinidine) and monoethylglycine-xylidide, a metabolite of lidocaine. The technique is rapid and specific, and permits measurement of several compounds simultaneously, although structural isomers of metabolites cannot be differentiated.

Administration of a 50:50 mixture of specifically deuterated and unlabeled warfarin has been used to unambiguously detect mass spectral ions derived from the parent drug or its metabolites (*AA69*); a new metabolite, benzylic hydroxywarfarin, was identified in rat liver microsomal preparations and in human urine from methane, isobutane, and ammonia chemical ionization spectra. Fenselau et al. have described a GC/CIMS method for the identification of an active metabolite of the antitumor agent, cyclophosphamide, in blood plasma of patients under drug therapy (*AA28*). Although the metabolite, *N,N*-bis(2-chloroethyl)phosphorodiamidic acid, could be determined in urine samples by EI mass chromatography, interference from other lipophilic material necessitated use of the CI technique for plasma extracts.

The quantitation of the oral hypoglycemic agent phenformin has been achieved by GC/CIMS following trifluoroacetic anhydride cyclization to the corresponding diamino-*S*-triazine (*AA56*). Using a deuterated analogue as an internal standard, the plasma level/time profile was obtained following oral administration of 100 mg of phenformin to a fasting diabetic

patient. Comparison with plasma glucose levels showed a decline in blood glucose during the rise of plasma phenformin levels; further investigation of this effect together with metabolite profiles is proposed. Plasma levels of another oral hypoglycemic agent, tolbutamide, and its metabolites have been monitored following intravenous administration to a diabetic patient using a similar CI technique (*AA57*). Direct sample introduction of the methylated sulfonylureas produced comparable results to gas chromatographic introduction despite partial cleavage of these compounds with the latter inlet method.

Urine concentrations as low as 5 ng/ml have been determined for morphine standard using mass chromatography with a GC/CIMS instrument (*AA18*), and 77 ng/ml were detected in the urine of a suspected drug user who had ingested a codeine-containing cough medicine. Codeine itself was found to be present in substantial amounts and is presumably the metabolic precursor of the detected morphine. High resolution and chemical ionization mass spectra have been used to identify normorphine and norcodeine as urinary metabolites of morphine after isolation by preparative thin layer chromatography (*AA8*).

Lin et al. have reported the measurement of phenacyclidine in blood and urine samples from intoxicated hospitalized patients (*AA53*); a concentration of 1 ng/ml of body fluid could be determined by GC/CIMS with selected ion monitoring.

The use of field ionization mass spectrometry has been described for the determination of methaqualone and 6-hydroxymethaqualone in human urine samples (*AA58*); a sensitivity limit of 200 pg/ml was reported by the use of standards multiply-labeled with deuterium.

A series of publications by Horning et al. has appeared describing the use of a GC/MS/computer system for drug studies in humans. Carbon-13 or deuterium-labeled analogues of diphenylhydantoin, phenobarbital, and valium were used as internal reference compounds for quantitation of these drugs in human plasma (*AA42*); the GC/MS analyses used methane chemical ionization or selected ion monitoring techniques, the latter method allowing detection in the picogram to nanogram range. Evaluation of negative ion chemical ionization at atmospheric pressure showed a detection limit of 30–50 femtograms of a drug standard injected directly into the source. Similar analyses are reported for several anticonvulsant drugs used in epilepsy treatment (*AA39*) by monitoring levels from 100–200 ml of plasma, 5–7 ml of urine, and 0.5–1.0 ml of breast milk. Time profiles can provide clinical information on patients who still have seizures while under treatment, and on mother–infant transfer of phenobarbital through breast-feeding. The kinetic parameters of various drugs and their metabolites have been determined (*AA41*) and would be useful in determining the rate-limiting step in specific drug metabolic pathways; other publications discuss applications in toxicology and neonatal pharmacology (*AA38, AA40, AA43*).

Many reports have appeared on structure identification and metabolic determinations in human physiological fluids by electron impact mass spectrometry; these include drug-types, such as antidepressants and hypnotics (*AA4, AA13, AA85*), barbiturates (*AA32, AA33, AA35*), anticonvulsant/antiepileptics (*AA52, AA55, AA63, AA70*), antitumor agents (*AA49, AA77*), anesthetics (*AA19, AA87*), antibiotics (*AA14, AA64*), and analgesics (*AA1, AA46*), as well as cardiac glycosides (*AA34*), hypertension drugs (*AA37, AA89*), a narcotic antagonist (*AA86*), and the antimalarial drug "Primaguine" (*AA3*).

The rapid identification of drugs and their metabolites by mass spectral methods has led to a routine analytical system for physiological fluids of overdose victims described by Costello et al. (*AA21*). Gas chromatographic retention indices are used in parallel with mass spectra for added specificity and are particularly useful for differentiating compounds having similar fragmentation patterns. The computer-searchable library contains mass spectra of normal body-fluid components and common contaminants in addition to drugs and their metabolites, and provides specific identifications in the absence of prior knowledge of compound class.

Stillwell et al. (*AA82*) have described the quantitation of the contraceptive steroid norethisterone in human plasma at the nanogram level following oral administration of 1 mg of the drug. By monitoring concentrations at various times after administration, the rate of metabolism was found to be relatively rapid but may vary because of differences in absorption rates. A study of the dose response relationship of methyl phenidate used in treating hyperkinetic children has been undertaken (*AA60*) using a GC/MS assay of the drug and its major metabolite, ritalinic acid, in blood and urine samples; concentrations of 10 ng/ml could be detected in subjects, and time-profiles of hyperactive children receiving daily medication indicate that measurable steady-state levels of both compounds should be considered in future treatment studies. The thermal decomposition of methylphenidate in the gas chromatograph injection port has been investigated in view of inconsistencies in previously published mass spectra (*AA29*); derivatization with trifluoroacetic anhydride is recommended for further studies.

Oral administration of a mixture of unlabeled and $^{15}N$-labeled Mydocalm, a central-acting muscle relaxant, was used to determine serum levels by GC/MS using a deca-deuterated analogue as an internal standard (*AA62*).

Stereoselective metabolism of RS-ibuprofen (2-[4-isobutylphenyl]propionic acid) was demonstrated by Brooks and Gilbert (*AA15*) by gas chromatographic resolution of the corresponding diastereomeric amides formed with R-(+)-$\alpha$-phenylethylamine; mass spectral data for the drug and identified urinary metabolites are reported. Ehrsson used GC/MS to identify the diastereomeric urinary metabolites of (±)-propranolol formed by conjugation with optically active $\beta$-D-glucuronic acid (*AA24*).

The active compound in cannabis preparations, $\Delta^9$-tetrahydrocannabinol, has been determined in plasma by mass chromatography (*AA73*) and in saliva by mass spectral analysis of thin layer chromatographic fractions (*AA50*). The specificity of mass chromatography has been used to unambiguously quantitate ethanol in human blood and urine (*AA66*), permitting rapid and reliable determinations of as little as 5 ng. Deuterated 4-methylpyrazol was used as an internal standard for GC/MS quantitation of the drug in human serum (*AA7*); 4-methylpyrazol is of potential clinical interest as it causes partial inhibition of ethanol oxidation in man.

Sullivan et al. have reported a mass chromatographic determination of methadone in human plasma with a sensitivity limit of about 16 pmol/ml (*AA83*); the method was used in a study of the pharmacokinetics in opiate-dependent subjects in which the maintenance does of methadone was replaced by an equivalent dose of $d_3$-methadone.

Free and conjugated methaqualone metabolites have been identified in urine, blood, and liver from three suicide cases (*AA9*). The sedative/hypnotic, glutethimide, has been responsible for many cases of serious intoxication due to acute overdoses and an accurate gas chromatographic assay with mass spectral confirmations has been applied to plasma samples from patients and to postmortem tissues (*AA36*).

In addition to drug identifications in humans, many papers have appeared on the mass spectral characterization (*AA45, AA81*) of reference standards and of metabolites isolated from animal studies; the utility of many of these investigations will no doubt be extended to human studies in the near future.

Chemical ionization mass spectra have been reported for tolbutamide (*AA51*), heroin preparations (*AA17*), and morphine and tropane alkaloids (*AA47*). Using methane as a reagent gas and direct sample introduction with repetitive scanning, tolbutamide (an oral hypoglycemic agent) could be determined from the quasimolecular (M + 1) ion derived from the intact compound (*AA17*), and quantitative measurements using the dideuteriobutyl analogue as an internal standard were reported for rabbit plasma levels following intravenous administration. The direct identification of heroin and many common diluents in powders can be achieved without prior sample treatment by CI mass spectrometry with proton transfer from isobutane (*AA17*); simple fragmentation patterns and, hence, fast interpretation provide a rapid screening or confirmatory method.

The oral anticoagulant phenprocoumon (which is related to warfarin) has been investigated by thin layer chromatography, ultraviolet absorption, and mass spectral methods (*AA68*); isobutane chemical ionization spectra are summarized for all the possible aromatic monohydroxylated derivatives synthesized as potential metabolites, in addition to the parent drug.

Jardine and Fenselau have studied a variety of pharmacologically active alkaloids by chemical ionization using nitric oxide diluted with nitrogen (*AA47*). In contrast to their isobutane chemical ionization spectra, all these compounds including heroin and morphine gave spectra in which the base peak corresponded to molecular ions; a comparison of EI and CI spectra using both nitric oxide in nitrogen and isobutane has been reported for constituents of an illicit heroin preparation (*AA48*).

Nelson et al. have reported the use of high resolution chemical and electron impact ionization mass spectrometry for the structural elucidation of medicinal carbamates (*AA65*); the techniques provide complementary information providing elemental compositions of base peak (M + H) ions from CI spectra, and detailed structural information from EI fragment ions. CI studies have also been described for the antibiotics lincomycin and clindamycin, which are active against many gram-positive pathogens (*A44*), and for penicillins and cephalosporins (*AA61*).

The utility of field desorption mass spectrometry (see section on FI and FD) for the identification of drugs has received some attention. Schulten (*AA79*) has reported the FD spectra of the antitumor drug cyclophosphamide and some of its metabolites at low and high (>15 000) resolution. Molecular weight information and the fragmentations induced at higher emitter heating currents are discussed; the availability of accurate mass measurements (errors ~10 ppm) permits interpretation of spectra derived from mixtures using photographic detection.

Azathioprine, an immunosuppressive agent widely used in organ transplantation therapy, and its metabolites have been studied by electron impact and field desorption ionization methods at both low and high resolution (*AA12*). One of the metabolites was isolated from rat urine following an oral dose of azathioprine and, after purification, gave a low resolution field desorption spectrum containing only intense M and (M + 1) ions. A similar comparison of FD and EI spectra was undertaken for ten carbamates which act as skeletal muscle relaxants and weak tranquilizers (*AA74*). Emylcamate did not produce a field desorption spectrum under various conditions and high volatility was suspected as the cause. Molecular or quasimolecular ions were abundant except for bethanechol chloride which gave a spectrum characteristic of compounds containing the quaternary ammonium group; however, no general diagnostic fragmentation could be determined for the carbamate function in the FD spectra of these molecules. Rinehart et al. have described the applicability of the field desorption technique for molecular weight determinations of nonvolatile or thermally unstable antibiotics including complexes such as streptovaricin, filipin, and dermostatin (*AA72*), and a comparison of the FD and EI spectra of rifamycins has been reported (*AA90*).

Electron impact ionization spectra are reported for several drugs and their metabolites, including investigations on promazine and promazine sulfoxide metabolites of phenothiazines using synthetic deuterated derivatives (*AA43*), aliphatic amine *N*-oxides and parent amines with structural features related to several drugs (*AA27*), aza-analogues of methaqualone (*AA67*), the vasodilating agent LS-121 (*AA84*), monoamine oxidase inhibitors (*AA22*), and 1,4-benzodiazepines (*AA71*). The identification of metabolites following administration of isotopically labeled drugs has been undertaken for $^{14}C$-labeled mescaline (*AA80*), a deuterated analogue of the antitumor agent cyclophosphamide (*AA20*), and deuterated digitoxigenin (*AA16*).

The mass spectral fragmentations of mepirizole (an analgesic and antiinflammatory agent) have been studied using deuterated analogues, and applied to the structure elucidation of metabolites isolated from rat urine (*AA78*). Accurate mass measurements were utilized in fragmentation studies of phenylbutazone (*AA75*), methylated tolbutamide derivatives by GC/MS (*AA76*), primaclone, glutethimide, and phenobarbital (*AA10*), and medicinal pyrazolidinediones (*A54*).

Sample introduction via a gas chromatograph has been used in studies of trimethylsilyl derivatives of various medicinal barbiturates (*AA25*), in the determination of methaqualone, phendimetrazine, and phenmetrazine in samples of street drugs (*AA11*), and for metabolites of the antitrichomonal drug 1-methyl-5-nitro-2-(2′-pyrimidyl)imidazole (*AA2*). A rapid quantitative procedure for trifluoroacetylation prior to GC/MS analysis of amphetamines is described, allowing derivatization of the free amine as well as the salt (*AA88*). Two *in vitro* metabolites of 3,4-methylenedioxyamphetamine, a common street drug, have been identified (*AA59*), and the quantitative determination of piribedil by mass fragmentography with an internal standard is reported to detect concentrations of 10 ng/ml or 10 ng/gm in biological samples (*AA26*).

The site of metabolic hydroxylation of cannabinoids can be determined by GC/MS of trimethylsilyl derivatives (*AA6*), and the determination of trazodone in rat plasma is described by a GC/MS method using benperidol as an internal standard (*AA5*). Using mass fragmentography to monitor two ions, a detectable limit of 200 pg of trazodone was achieved, and the pharmacokinetics in rat plasma following a single intravenous dose is described.

Gal et al. (*AA30*) have investigated the *N*-hydroxylated metabolites of a potent psychotomimetic amphetamine derivative using rabbit liver microsomal preparations; GC/MS analyses of trifluoroacetyl derivatives were undertaken on the products obtained from incubations of 1-(2,5-dimethoxy-4-methylphenyl)-2-aminopropane and a deuterated analogue, and quantitation of deuterated metabolites of the deuterated amine by selected ion monitoring utilized the nondeuterated analogue as an internal standard.

## APPLICATIONS IN ENVIRONMENTAL CHEMISTRY

The study of organic compounds in the environment is a complex subject and encompasses the nature and fate of "natural" compounds as well as pollutants created by the activities of man. A recent volume in the "Specialist Periodical Reports" series summarizes many of the fields of research with particular emphasis on aquatic environments (*AB29*). The chromatographic separations necessary prior to mass spectrometric analysis have formed the subject of recent books by Fishbein (*AB37*) and Grob (*AB50*), and a general review on methodology for pesticide residue analysis has appeared (*AB102*).

The significant role of mass spectrometry in the field of pesticide chemistry is exemplified in the book edited by Haque and Biros (*AB52*), which compiles the symposium papers presented during the 165th ACS National Meeting in April 1973. Coverage includes the EI and CI mass spectra of metabolites of DDT-type pesticides, the positive and negative chemical ionization spectra of polychlorinated pesticides, ion kinetic energy spectra of isomeric chlorophenols, determination of metastable transitions in pesticide mass spectra, and the identification of organophosphate insecticides, nitroaniline-derived herbicides and insecticide photoproducts.

Several general papers have appeared emphasizing the utility of mass spectral methods (*AB16, AB17, AB35, AB83*) and associated computer techniques (*AB2, AB55, AB62*) for environmental studies. Oswald et al. (*AB88*) have published a detailed review containing over 300 references on the use of GC/MS with electron impact and chemical ionization in the study of environmental health problems, and cover the characterization of natural product agents (hydrocarbons, essential oils, etc.), as well as man-made chemicals such as chlorinated hydrocarbons and plasticizers. A recent review by Alford (*AB1*) cites nearly 400 references covering the period 1969–1974 with emphasis on the types of pollutants identified in environmental samples by organic and spark source mass spectrometry. The majority of reports on mass spectral investigations of trace organic species in air and water utilize GC/MS combination methods and, in general, new techniques specific to these studies are primarily concerned with sample preconcentration and introduction into the gas chromatograph; current methodology in this area has recently been reviewed in detail (*AB20*). Sampling considerations have been discussed by Bertsch et al. (*AB8*) who utilized capillary column GC/MS for the study of volatiles in industrial and urban environments; approximately 100 components have been identified in the air samples, mainly normal and branched alkanes and alkylated benzenes.

A portable quadrupole mass spectrometer/computer system has been developed for monitoring organic vapors (*AB33*); the instrument incorporates an inlet system comprised of two Llewellyn silicone membrane 3-stage separators providing a

sample enrichment of about $10^6$. Hollow fiber probes have been described for high sensitivity analyses of trace volatile contaminants in aqueous solution and in air (*C65*). Perry and Twi ll (*AB92*) have measured benzene and other hydrocarbons in London street air using a timed elution procedure which eliminated interference from cryogenically-condensed water vapor and the use of solvents. Using background subtraction and a 14-amu library search routine, quantities down to about 20 ng could be identified, which corresponded to a concentration of ~110 μg benzene/$m^3$ street air for a 9-l. sample. An additional (preparative) gas chromatograph was used by Tyson and Carle for the separation of water from cryogenically collected air samples prior to the analytical GC and MS (*AB117*).

Bergert et al. (*AB6*) have reported the identification of 20 components in air samples in Frankfurt am Main using glass capillary GC/MS; the compounds included acetone, $C_8$–$C_{11}$ *n*-alkanes, monoaromatic hydrocarbons, and chlorinated derivatives of methane, ethylene, and benzene. A similar analysis of room air (*AB4*) identified methanol, acetone, diethylether, methyl acetate, chloro-ethylenes, hexane, and monoaromatic hydrocarbons.

Several papers describe the detection of chlorinated species in air, also by GC/MS methods. A detection limit of less than $10^{-2}$ ppb has been reported for bis(chloromethyl)ether in a 1-l. air sample using single ion monitoring; with multiple ion monitoring for increased specificity, threshold limits of 1 and 10 ppb were estimated for bis(chloromethyl)ether and dimethylsulfate, respectively. Levels of 0.1 ppb and 0.01 ppb v/v) have been reported by Evans et al. for bis(chloromethyl)ether in 1- and 10-l. air samples, respectively (*AB34*). This method uses monitoring of the GC effluent at a mass resolution of 3800 ($C_2H_4OCl^+$ = *m/e* 78.9950) and thus provides a significant increase in compound specificity; the relative effects of static and dynamic monitoring are discussed. Grimsrud and Rasmussen used direct GC/MS coupling together with high-speed pumping and single ion monitoring for the quantitative analysis of $CFCl_3$ and $CF_2Cl_2$ in rural air samples collected in Washington State (*AB48*); the detection limit was estimated to be about 5 ppt ($5 \times 10^{-12}$ v/v) or about 0.5 pg/20 $cm^3$. The method was extended to several specific atmospheric halocarbons (*AB49*) including methyl chloride which was found in relatively large concentrations (530 ± 30 ppt) in the same area.

Schultz et al. (*AB109*) have published a detailed investigation of the organic material in airborne particulate matter in samples collected near power stations and major airports, and in urban areas; the results were compared with data obtained from possible pollution sources (jet engine exhausts, jet and diesel fuels, and a condensate from the effluent of a coal-combustor). These studies utilized direct sample vaporization and accurate mass measurement at a resolution of 12 000, and permitted evaluation of carbon number distribution and of C:H ratios (which distinguished aliphatic and aromatic components) for each sample.

Diesel exhaust particulates have also been studied using capillary column GC/MS subsequent to column chromatographic fractionation of organic extracts (*AB72*), and alkanes, polycyclic aromatic hydrocarbons, and phenolic components were identified. Boyer and Laitinen investigated the ether extracts of automobile exhaust particulates by GC/MS of column chromatographic fractions (*AB15*) using mass chromatograms to locate components of interest in the resulting complex mixtures; the effects of UV irradiation and lead halides on the organic material associated with particulates were evaluated. High resolution mass spectrometry at low ionizing voltage is reported for the detection of polycyclic aromatic hydrocarbons in dust samples collected from cities and near highways (*AB56*), and a method for the determination of polycyclic quinones in particulates utilized UV, luminescence, and mass spectral analyses (*AB93*). Gas chromatographic fractionation followed by rechromatography on a capillary column GC/MS system was used to identify polar and nonpolar constituents of fresh tobacco smoke including aldehydes, ketones, and nitriles (*AB10*).

Qualitative and quantitative information on atmospheric aerosols has been obtained by computer-controlled mass spectrometry at a resolution of 10 000 (*AB107*); the method utilized a compound reference library based on accurate masses and relative intensities of the molecular ion and three additional ions, together with chromatographic retention times relative to standards. Components discussed include inorganic oxides and sulfates, inorganic and organic halides and nitrates, alkyl-benzenes and -phenols, and polycyclic aromatics.

Additional studies in this area include GC/MS analysis of volatile organics in the cabin atmosphere of Skylab 4 (*AB9*) and the effect of organic vapors on the clustering of $H_3O^+(H_2O)_n$ ions in the troposphere (*AB64*). The analysis of aerosols produced by the ozonolysis of 1-butene has been investigated with high resolution field desorption mass spectrometry (*AB108*; see also FD portion of Ion Chemistry section) and reported data include an evaluation of mass measurement accuracy as a function of mass (*m/e* 30–220), using a field ionization spectrum of perfluorotributylamine as a reference.

The mass spectrometric identification of organic species in water samples has received increasing attention in recent years. Many of the procedures used may be found in series of research reports from the Office of Research and Development of the U.S. Environmental Protection Agency, and include the evaluation of resins, foams, and solvent extraction for isolating organic water pollutants (*AB119*), and recommended procedures for the application of GC/MS to wastewater analyses (*AB120*).

Harris et al. (*AB53*) have explored the use of direct aqueous injection for GC/MS analyses using a quadrupole mass spectrometer; the effects of relatively large pressures of water vapor were evaluated with respect to system performance and the electron impact fragmentation patterns. The detection limit under scanning conditions (~1 mg/l.) is compatible with the concentrations of organics found in domestic sewage and wastewater effluents, but monitoring of selected ions allowed concentrations of the order of 100 ppb to be detected for analyses of clean surface waters and drinking water.

The use of chemical ionization mass spectrometry (see CI portion of Ion Chemistry section) has been reported by Price et al. (*AB94*), with direct injection of dilute aqueous solutions (15–30 μl) into a heated 1-l. batch inlet system. The water provided the reagent gas, the principal reactant ions being $H_3O^+(H_2O)_n$ ($n$ = 0–5), and the spectra obtained for aniline, valeronitrile, acetone, and diethyl ether were evaluated.

Concentration of aqueous samples by gas phase stripping prior to glass capillary GC/MS has been described for the determination of volatile organics in aqueous solution (*AB6*, *AB7*); the latter paper evaluates TENAX GC for absorption prior to separation and analysis, and reports components identified in city drinking waters and natural river water.

Several papers have appeared on the use of mass spectrometry for the investigation of organic constituents in drinking waters, and a bank of mass spectral data has been initiated in tabular form (*AB69*). Scheiman et al. found aliphatic and aromatic hydrocarbons, chlorocarbons, alcohols, ketones, and bromine-containing compounds in the water supply of the District of Columbia (*AB105*) following solvent extraction of 1-gallon samples.

Several halocarbons were identified in New Orleans drinking water (*AB27*) and, in the same study, carbon tetrachloride, tetrachloroethylene, and isomers of dichlorobenzene were found to be present in blood plasma obtained from local residents. Additional investigations have been reported on the analysis of aromatic and halogenated aliphatic hydrocarbons in the original water source and at various stages of a water treatment process (*AB26*). Mass spectral identification was utilized in a study of the formation of haloforms—apparently by the haloform reaction—during chlorination of natural waters (*AB99*) and in the determination of an odorous compound (geosmin) in the raw water of public water supplies (*AB76*).

A comprehensive report on the organic content of finished drinking waters from thirteen U.S. cities has been compiled by Keith et al. (*AB75*) and contains details of methodology including GC/MS with packed and glass capillary columns, methane-CI mass spectrometry of GC effluents, and some high resolution mass measurements. Samples were obtained by carbon filtration followed by clooroform extraction and concentration so that 1 μl of the final extract corresponded to 1 l. of water; a total of 109 different compounds were identified in the extracts including pesticides, herbicides, aliphatic and aromatic hydrocarbons, halogenated aliphatics, chlori-

nated aromatics, and plasticizers.

A variety of organic compounds (aliphatic and aromatic hydrocarbons, fatty acids, phthalates, and sterols) have been identified by GC/MS in water samples from the polluted Tamagawa River in Japan (*AB66, AB85*). The contamination of water with plasticizers and other polymer additives derived from various synthetic polymer tubes has also been reported (*AB70*).

Several studies have been undertaken on the organic components of municipal and industrial wastewaters such as sewage plant effluents (*AB94*) and pulp mill discharges (*AB63*). Keith (*AB74*) has reported the characterization of wastewaters discharged into the Calcasieu River, Louisiana, from petrochemical, petrorefinery, synthetic rubber, and chemical plants; the investigation revealed the discharge of chemicals not previously listed by the manufacturers.

Glass capillary GC/HRMS (see section on GC/MS/on-line computer techniques) has been utilized in studies of complex mixtures derived from secondary effluents of a sewage treatment plant (*AB19*) and from various stages throughout the water treatment scheme of a petroleum refinery (*AB18*). The use of elemental composition (accurate mass) chromatograms enabled specific components to be located and identified even though the complexity of the mixtures precluded recognition from GC profiles or total ionization chromatograms. The identification of saturated fatty acids, *n*-alkanes, alkylbenzenes, and higher aromatic hydrocarbons has been reported in ether extracts of secondary effluents by GC/MS (*AB82*), and a study of the effects of chlorination on the organic components of secondary municipal wastewater effluents utilized GC/MS methods (*AB46, AB47*).

Several publications have appeared on the identification of polycyclic aromatic hydrocarbons in environmental samples by mass spectrometric methods. Giger and Blumer have described an isolation procedure (gel filtration, adsorption chromatography, and charge transfer complexation) which provided concentrates of various aromatic ring-types which were analyzed by UV and mass spectrometry using programmed temperature probe distillation and 12-eV electron beam energy (*AB44*). Volatility profiles and ion series plots contributed to the characterization of the complex mixtures obtained from soils and sediments (*AB11*). GC/MS has been used for the identification of these hydrocarbons in industrial effluents, coke oven emissions, coal tar, and airborne particulates (*AB78*), and quantitation was achieved by computerized gas chromatography using fluoranthene as the internal standard.

Giger et al. have characterized polycyclic aromatic hydrocarbons in samples of domestic sewage, diesel fuel, and an oil-contaminated recent sediment (*AB45*), and have investigated the effect of aqueous chlorination on the aromatic fraction of diesel fuel (*AB97*). The latter study utilized a glass capillary column coupled directly to the mass spectrometer ion source via platinum capillary tubing, and the resulting mass chromatograms were processed by specific additions and subtractions to provide a selective method for searching for mono- and dichlorinated species.

The analysis of chlorinated organics in environmental samples is of considerable interest in view of the known or potential toxicity of numerous manmade pollutants of this type, and their persistence and accumulation in biological organisms. In addition to the numerous identifications of these compounds and their metabolites and photodecomposition products by mass spectral—generally GC/MS—methods (*AB1, B20*), several publications have appeared which emphasize new or unusual techniques. Dzidic et al. used chemical ionization at atmospheric pressure in a study of the negative ions formed from chlorinated aromatic compounds (*AB28*); nitrogen (containing ~0.5 ppm oxygen) or air were used as carrier gases, and the temperature and pressure conditions simulated those of an electron capture GC detector. The formation of phenoxide ions by ion–molecule reactions involving oxygen was investigated, and the detection of 150 femtograms of 2,4,5,6-pentachlorobiphenyl was achieved by monitoring the tetrachlorophenoxide ion at *m/e* 307. As the sensitivity of this technique is comparable to that of electron capture detection, and the structural specificity much greater, its use in the trace detection and quantitation of chloroaromatics is recommended.

GC/MS with electron impact and chemical ionization has been described for the differentiation and characterization of isomeric polychlorinated biphenyls (PCB's) (*AB89*). A comparison of the EI spectra of model compounds was undertaken and the relative abundance of $(M - Cl)^+$ ions was found to be of value in the differentiation of isomers of di-, hexa-, and hepta-chlorinated PCB's using "limited range" mass chromatograms. Eichelberger et al. (*AB32*), report a "subset data acquisition" technique for PCB analyses using a computer-controlled quadrupole mass spectrometer coupled to a gas chromatograph for monitoring ions characteristic of mono- to hexa-chlorobiphenyls. High resolution mass spectrometry with photoplate detection has been utilized for screening PCB metabolites in rabbit and goat urines (*AB65*).

The chromatographic and biological aspects of DDT [1,1,1-trichloro-2,2-bis(*p*-chlorophenyl)ethane] have been reviewed by Fishbein (*AB36*). Dougherty et al. have investigated CI mass spectrometry for the direct analysis of this class of pesticides (*AB25*); both positive and negative ion CI spectra were recorded using isobutane as the reagent gas, the former spectra showing high intensity ions (often the base peak) corresponding to $(M - Cl)^+$, whereas the negative ion spectra were characterized by intense $(M + Cl)^-$ anions.

The analysis of polychlorinated dibenzofurans and dibenzo-*p*-dioxins by mass spectral methods has received significant attention. Safe et al. recorded both the ion kinetic energy and mass spectra of several chlorinated dibenzo-*p*-dioxins in a study of the decomposition pathways induced by electron impact ionization (*AB103*). The IKE technique yielded distinctive spectra for all the isomers studied and, despite present sensitivity limitations, may prove to be an additional analytical tool. A time-averaged high resolution mass spectrometric technique has been described by Baughman and Meselson for the detection of tetrachlorodibenzo-*p*-dioxin at the picogram level (*AB5*); rapid scanning over a very limited mass range was achieved by deflecting the beam over the detector slit with a small additional magnetic field. The method was evaluated in terms of possible interference from other chloroorganics, and the size and nature of the total sample to be analyzed. In connection with a proposed pharmacokinetic study of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin using isotopically-labeled standards and dual ion monitoring, Reynolds and Delongchamp have calculated the theoretical isotopic abundances and optimum dwell times for the analysis of this compound by negative ion CI at atmospheric pressure (*AB98*).

The use of CI mass spectrometry has been evaluated for organophosphorus (*AB60*) and *N*-methylcarbamate insecticides and their metabolites (*AB59*), and the effect of chemical structure on the fragmentation patterns obtained using methane or perdeuteriomethane reagent gases is discussed. Methane CI mass spectra obtained from gas chromatographic effluents were used in a study of toxaphene, an insecticide produced by the catalytic and photolytic chlorination of camphene (*AB61*). This method revealed a complex mixture containing more than 177 polychlorinated $C_{10}$ components.

The identification of the volatilizable and/or solvent-extractable components in polymers is of interest not only because of environmental considerations, but also because these components may occur in mixtures due to improper sample handling and storage. Sigmond has reported a mass spectrometric method for the volatile substances in elastomers and plastics intended for high vacuum use (*AB111*). Samples were introduced directly into the ion source and low or high (~10 000) resolution mass spectra were obtained during volatilization. Much of the data is presented as low resolution "mass integrated" spectra in which the ordinate at a specific *m/e* value, $M_i$, represents the integrated ion current due to all ions $\geq M_i$; single prominent masses appear as steps in the resulting profile. Materials tested included Araldite, nylon, polyethylenes, polyimide (Vespel), polypropylenes, Teflon, neoprene, silicone rubbers, and Viton.

The use of plasma chromatography and mass spectrometry has been described for the identification of isomeric phthalic acids which, along with derivatives, are used as plasticizers in polymeric packaging materials (*AB71*); the paper presents some positive and negative ion EI spectra and methane CI spectra, and these methods for the differentiation of isomers are compared. The plastcizer di-(2-ethylhexyl)phthalate was identified by GC/MS in the condensate obtained by pyrolysis of a polyvinyl chloride meat wrapping film (*AB67*), and mass

chromatographic methods for the analysis of vinyl chloride in foods have been reported (*AB100, AB121*). A quinone product obtained from the autoxidation (two years at room temperature) of the antioxidant 2,6-di(*tert*-butyl)-4-methylphenol in a commercial polyethylene film has been identified (*AB22*), and GC/MS was used in a study of the impurities in 4,4'-dichlorodiphenyl sulfone, a reagent in the manufacturing of polysulfone thermoplastics (*AB43*).

The identification of polycyclic aromatic hydrocarbons in environmental samples (see above) is directly related to many of the studies undertaken by organic geochemists and petroleum chemists. Many of the current topics of interest in these fields—which often utilize mass spectrometric analyses—may be found in the proceedings of the International Meetings on Organic Geochemistry, held in France in September 1973 (*AB115*) and in Madrid in September 1975 (*AB87*).

The overlap between pollution studies and organic geochemistry has been pointed out by Eglinton et al. (*AB31*): "certain alkanes, cycloalkanes, and aromatic hydrocarbons may enter the environment naturally by way of oil seeps and erosion of sedimentary deposits, by contemporary biosynthesis, or as the result of industrial processes. The same compound can have multiple origins." This publication discusses the recognition of organic pollutants in aquatic sediments and describes the utilization of computerized GC/MS methods to identify phthalate esters, polycycylic aromatic hydrocarbons, and partially degraded crude oil in an estuarine sediment. Mass spectrometric analyses of polycyclic aromatic hydrocarbons in soils and recent marine sediments have been reported (*AB11, AB44, AB122*) and the nature and distribution of alkanes at the air–sea interface from off-shore Louisiana and Florida have been described (*AB80*). Other mass spectral studies relating to marine pollution include the use of field ionization mass spectrometry for fingerprinting mineral oils (*AB68*, p 229), GC/MS analyses of No. 2 fuel oil added to pre-extracted estuarine water (*AB68*, p 149), and the hydrocarbon composition of extracts of lake and coastal sediments (*AB68*, p 217).

The occurrence of tetra- and pentacyclic hydrocarbons (steranes and triterpanes derived from biologically-occurring triterpenoids) in oil shales and kerogen has been studied by GC/MS methods. Kimble et al. have evaluated the mass spectrometric and high resolution gas chromatographic behavior of a variety of structural types of authentic steranes and triterpanes (*AB77*) and have identified many such compounds in an Eocene oil shale (*AB78, AB118*). Two triterpanes, shionane and friedelane, were included in a study of the characteristic fragmentation patterns of their derivatives by high resolution mass spectrometry (*AB58*). The pyrolytic release of steranes and terpanes from Green River Formation oil shale kerogen has been reported (*AB41*), and identifications were made by pyrolysis/GC/MS and by GC/MS of fractions of pyrolysate obtained by column chromatography. Rearranged sterenes (monounsaturated steranes) have been identified in an 180-million-year-old clay-rich sediment of marine origin (*AB101*), and mass chromatography of trimethylsilyl derivatives was used to study stanols in lake sediment cores (*AB86*).

Hertz et al. have reported a GC/MS method for the analysis of volatile hydrocarbons at the ppb level (*AB57*); the procedure involves dynamic headspace sampling and was utilized in studies of intertidal zone sediments from the Northeastern Gulf of Alaska.

The analysis of petroleum and crude oils by mass spectrometry has continued to receive attention. Lumpkin et al. have described the use of dynamic scanning at a resolution of >70 000 for the study of sulfur-containing petroleum fractions (*AB81*). Mass chromatographic data were used to identify components of a pyrolysis naphtha separated by capillary column gas chromatography (*AB42*), and the technique was extended for the detection of sulfur-containing compounds by monitoring the $CHS^+$ ion at a resolution of ~2000 (*AB40*). Fisher and Fischer have described the quantitative analysis of petroleum streams by obtaining accurate mass measurements from slow scanning at 10 000 resolution (*AB38, AB39*), and a method for the high pressure sampling and mass spectrometric analysis of gasoline streams is reported (*AB96*).

In addition to hydrocarbons, studies on oxygen- and nitrogen-containing compounds have been undertaken. The progress made in the structural elucidation of carboxylic acids in petroleum and sediments has been reviewed by Seifert (*AB110*). Cranwell used GC/MS to identify branched and cyclic monocarboxylic acid methyl esters isolated from lake sediments and discussed the value of this compound class in the assessment of paleoenvironmental trophic levels (*AB21*). Capillary column GC/MS was used by Boon et al. in a study of the monocarboxylic fatty acids (*AB13*) and hydroxy acids (*AB12*) isolated from sediments consisting of diatomaceous microfossils, and phytenic acids have been identified in the same sediments and in the detritus of an unpolluted lake (*AB14*). A variety of polar components isolated from Green River Formation oil shale have been characterized by IR, NMR, and mass spectrometric techniques (*AB3*); the compound types reported include cyclohexanols, isoprenoid ketones, tetralones and indanones, tetrahydroquinolines, quinolines, alkoxypyrrolines, and maleimides. The relative abundances of homologous petroporphyrins have been measured by mass spectrometry in samples of crude oils and their presumed source rocks (*AB24*), and a detailed structural characterization of crude oil petroporphyrins utilized GC/MS identification of maleimides derived by controlled oxidative degradation (*AB23*).

A new calibration matrix has been reported for the compositional analysis of coal liquefaction products by low resolution mass spectrometry (*AB113*); the method differs from those used for petroleum and utilizes the fact that coal liquids contain relatively short series of homologues of aromatic hydrocarbons. Hamming et al. have analyzed the volatiles from fresh coal surfaces by high resolution mass spectrometry using photoplate detection (*AB51*), and the organic components in bituminous coals from East Greenland have been studied by GC/MS (*AB90*).

The characterization of the chemical structure of humic substances also utilizes mass spectrometric methods for the identification of products derived from degradative experiments. Schnitzer and Skinner studied the products obtained from a humic and a fulvic acid following relatively mild oxidation with peracetic acid (*AB106*), and used mass chromatographic data for the identification of the major products from the hydrolysis of fulvic acid (*AB112*).

Mass spectrometry was used to study the conversion of triphenylamine to *N,N,N',N'*-tetraphenylbenzidine by complex formation with the clay mineral montmorillonite (*AB116*), and the formation of aniline is reported following pyrolysis of a diprotonated 4,4'-diaminostilbene/montmorillonite intercalate (*AB114*). Mass spectral data are reported for trimethylsilyloxy derivatives obtained by hydrochloric acid treatment of the silicate mineral natrolite (*AB30*), and for the products derived from the acid clay catalyzed dimerization of fatty acids (*AB84*).

Pereira et al. determined the concentrations of eight protein amino acids in aqueous extracts of the Murchison meteorite by mass chromatography with deuterated internal standards (*AB91*). Extraction with deuterium oxide resulted in some deuterium exchange in existing C–H bonds, rather than C–D synthesis during extraction; some degree of racemization of the amino acids was indicated in the process of deuterium incorporation from deuterium oxide.

## ACKNOWLEDGMENT

A bibliography of the Japanese literature during this period was kindly compiled for us by Makato Suzuki, Professor of Faculty of Pharmacy, Meijo University, Nagoya; he is an authority on the application of mass spectrometry to elucidation of the structures of macrolide antibiotics. We wish to mention helpful information from T. Baez, H. D. Beckey, I. Dzidic, C. Fenselau, E. and M. Horning, J. D. Morrison, and J. T. Watson. We thank Dan Kuklo who assisted with the literature search, and Maryann Aberg, Sherry Dobo, and Virginia Schutz for production of the manuscript. We gratefully acknowledge the support of the National Institutes of Health Research Grant RR 719-03 from the Division of Research Resources, the National Aeronautics and Space Administration Grant NGL 05-003-003, the National Science Foundation Grant MPS 72-05129A02, and the Environmental Protection Agency Grant R803984-01.

## LITERATURE CITED


### Overview

(A1) Biemann, K., *Origins of Life*, 5, 417 (1974)
(A2) Budde, W. L., *Biomed Mass Spectrom.*, 1, 427 (1974)
(A3) Lee, T., Papanastassiou, D. A., Wasserburg, G. J., *J. Geophys. Res. Lett.*, in press (1976).
(A4) Meyerson, S., *Biomed Mass Spectrom.*, 2, 59 (1975)
(A5) Nier, A. O., Hanson, W. B., McElroy, M. B., Seiff, A., Spencer, N. W., *Icarus*, 16, 74 (1972).
(A6) (a) Report to IUPAC Subcommission on Ion Monitoring Nomenclature Discussions at 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975. (b) Report on Ion Monitoring Nomenclature Discussions at 3rd International Symposium on Mass Spectrometry in Biochemistry and Medicine, Sardinia, 1975. (c) Report on Nomenclature Workshop at 2nd International Conference on Stable Isotopes, Argonne National Labs, Oakbrook, Ill., 1975.
(A7) Robertson, A. J. B., Ed., "Recommendations for Nomenclature of Mass Spectrometry", International Union of Pure and Applied Chemistry, Analytical Chemistry Division, Commission on Analytical Nomenclature, Butterworths, London, 1973, p 471.
(A8) Tera, F., Wasserburg, G. J., *Anal. Chem.*, 47, 2214 (1975).
(A9) Watson, J. T., Falkner, F. C., Sweetman, B. J., *Biomed. Mass. Spectrom.*, 1, 156 (1974).

### Scope of This Review

(B1) Alford, A., *Biomed. Mass Spectrom.*, 2, 229 (1975).
(B2) Ausloos, P., Ed., "Interaction between Ions and Molecules", Plenum Press, New York and London, 1975.
(B3) *Biomedical Mass Spectrometry*, Heydon & Son Ltd., London.
(B4) Burlingame, A. L., Cox, R. E., Derrick, P. J., *Anal Chem.*, 46, 248R (1974).
(B5) Chapman, J. R., "Computers in Mass Spectrometry", Academic Press, New York and London, 1976
(B6) Czanderna, A. W., "Methods of Surface Analysis", Methods and Phenomena, Vol. I, Elsevier Publishing Co., New York, 1975.
(B7) Elliott, R. M., Ed., "Advances in Mass Spectrometry", Vol. 2, Macmillan, New York, 1963.
(B8) Evans, C. A., Jr., *Thin Solid Films*, 19, 11 (1973).
(B9) Falkner, F. C., Sweetman, B. J., Watson, J. T., *Appl Spectrosc. Rev.*, 10, 51 (1975).
(B10) Frigerio, A., Castagnoli, N., Jr., Ed., "Mass Spectrometry in Biochemistry and Medicine", Raven Press, New York, 1974.
(B11) Green, M. M., in "Topics in Stereochemistry", Vol. 9, E. Eliel and N. Allinger, Ed., John Wiley & Sons, New York, 1975.
(B12) Heller, S. R., in "Computer Representation and Manipulation of Chemical Information", W. T. Wipke, S. R. Heller, R. J. Feldman, E. Hyde, Ed., John Wiley & Sons, New York, p 175.
(B13) Hesse, M., in "Progress in Mass Spectrometry", Vol. I, H. Budzikiewicz, Ed., Verlag Chemie, Weinheim/Bergstr., Germany, 1974.
(B14) Holmes, J. L., in "Isotopes in Organic Chemistry", Vol. 1, E. Buncel and C. C. Lee, Ed., Elsevier Scientific Publishing Co., Amsterdam, 1975, p 61.
(B15) *International Journal of Mass Spectrometry and Ion Physics*, Elsevier Publishing Co., Amsterdam.
(B16) Johnstone, R. A. W., Sr. Reporter, "Mass Spectrometry," Vol. 3, Specialist Periodical Report, The Chemical Society, London, 1975.
(B17) Keith, L. H., Ed., Proceedings of the Symposium on the Identification and Analysis of Organic Pollutants in Water, University of Michigan Press, Ann Arbor, Mich., in press.
(B18) Maccoll, A., Ed., "Mass Spectrometry", Int. Rev Science, Physical Chemistry, Series Two, Vol 5, Butterworths, London, and Boston, Mass., 1975.
(B19) Mandelbaum, A., "Handbook of Stereochemistry", H. Kagan, Ed., Georg-Thieme Verlag Stuttgart Publischen, Paris, in press.
(B20) *Mass Spectrometry Bulletin*, Mass Spectrometry Data Center, Aldermaston, United Kingdom.
(B21) *Mass Spectroscopy*, Mass Spectroscopy Society of Japan, Toyonaka, Japan.
(B22) Matsumoto, I., Ed., "GC/MS News", Kurume University, Japan, 1975.
(B23) McDowell, C. A., in "Methods of Experimental Physics: Vol. 3, Molecular Physics, Second Edition, Part B", D. Williams, Ed., Academic Press, New York and London, 1974, p 575.
(B24) Mead, W. L., "Advances in Mass Spectrometry", Vol. 3, Institute of Petroleum, London, 1966
(B25) Moore, R. H., Robinson, D., Argent, B. B., *J. Phys E*, 8, 641 (1975).
(B26) Nishiwaki, T., *Heterocycles*, 2, 473 (1974)
(B27) *Organic Mass Spectrometry*, Heydon & Son, London.
(B28) Raychaudhuri, P. K., Stafford, F. E., *Mater. Sci. & Eng.*, 20, 1 (1975).
(B29) Smith, D. H., Masinter, L. M., Sridharan, N. S., in "Computer Representation and Manipulation of Chemical Information", W. T. Wipke, S. R. Heller, R. J. Feldman, E. Hyde, Ed., John Wiley & Sons, New York, 1975, p 287.
(B30) Smith, K. M., in "Porphyrins and Metalloporphyrins", K. M. Smith, Ed., Elsevier Publishing Co., Amsterdam, 1975, p 381.
(B31) Stenhagen, E., Abrahamsson, S., McLafferty, F. W., Ed., "Registry of Mass Spectral Data", Vol. 1–4, John Wiley & Sons, New York, 1974.
(B32) Tatematsu, A., Miyazaki, H., Suzuki, M., "Practical Mass Spectrometry for Medical and Pharmaceutical Science", Kodansha Scientific, 1975, in Japanese.
(B33) Tissot, B., Bienner, F., Ed., "Advances in Organic Geochemistry 1973", Editions Technip, Paris, 1974.
(B34) Tsuchiya, T., "Gas Chromatography—Mass Spectrometry and its Application", Kodansha Scientific, 1974, in Japanese.
(B35) Vollmin, J. A., in "Clinical Biochemistry—Principles and Methods", H. Ch. Curtius and M. Roth, Ed., Walter de Gruyter, Berlin, 1974, p 753.
(B36) Waldron, J. D., Ed., "Advances in Mass Spectrometry", Vol. 1, Pergamon Press, New York/London, 1959.
(B37) Watson, J. T., "An Introduction to Mass Spectrometry: Biomedical, Environmental and Forensic Applications", Raven Press, New York, 1976.
(B38) West, A. R., Ed., "Advances in Mass Spectrometry", Vol. 6, Applied Science Publishers Ltd., London, 1974.
(B39) Wilson, R. G., "Ion Mass Spectra," Wiley-Interscience, N.Y., 1974.

### Innovative Techniques and Instrumentation

(C1) Anhalt, J. P., Fenselau, C., *Anal. Chem.*, 47, 219 (1975).
(C2) Bakale, D. K., Colby, B. N., Evans, C. A., Jr., *Anal. Chem.*, 47, 1532 (1975).
(C3) Beynon, J. H., Jones, D. O., Cooks, R. G., *Anal. Chem.*, 47, 1734 (1975).
(C4) Bibring, J. P., Borg, J., Burlingame, A. L., Langevin, Y., Maurette, M., *Proc. Sixth Lunar Sci. Conf., Geochim. Cosmochim. Acta, Suppl. 6*, 3, 3471 (1975).
(C5) Bibring, J. P., Burlingame, A. L., Chaumont, J., Langevin, Y., Maurette, M., Wazolek, P. C., *Proc. Fifth Lunar Sci. Conf., Geochim. Cosmochim. Acta, Suppl. 5*, 2, 1747 (1974).
(C6) Bonner, R. F., Lawson, G., Todd, J. F. J., March, R. E., in "Advances in Mass Spectrometry", Vol. 6, A. R. West, Ed., Applied Science Publishers Ltd., 1974, p 377.
(C7) Bridger, N. I., Craig, R. D., Sercombe, J. S. F., in "Advances in Mass Spectrometry", Vol. 6, A. R. West, Ed., Applied Science Publishers Ltd., 1974, p 365.
(C8) Brown, R. W., Lippiatt, J. H., Price, D., Izod, D. C. A., *Int. J. Mass Spectrom. Ion Phys.*, 16, 101 (1975).
(C9) Brubaker, T. A., Pomernacki, C. L., Brackett, H. B., Jr., *Proc. IEEE*, 63, 1467 (1975).
(C10) Carrick, A., Paisley, H. M., *Org. Mass Spectrom.*, 8, 229 (1974).
(C11) Chait, E. M., Hull, C. W., *Am. Lab.*, 7(6), 47 (1975).
(C12) Comisarow, M., Marshall, A. G., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, May 1975, p 453.
(C13) Cooks, R. G., Solka, B. H., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, May 1975, p 660.
(C14) Crowder, B. L., Ed., "Ion Implantation in Semiconductors and Other Materials", IBM Research Symposium Series, Plenum Press, New York-London, 1973.
(C15) Dawson, P. H., Lambert, C., *Int. J. Mass Spectrom. Ion Phys.*, 16, 269 (1975).
(C16) Dawson, P. H., Lambert, C., *Int. J. Mass Spectrom. Ion Phys.*, 14, 339 (1974).
(C17) Dawson, P. H., Whetten, N. R., *Res./Dev.*, 2, 46 (1968)
(C18) Dearnaley, G., Freeman, J. H., Nelson, R. S., Stephen, J., "Ion Implantation", Defects in Crystalline Solids Series, Vol 8, North-Holland Publishing Co., Amsterdam, 1973.
(C19) Donohue, D. L., Harrison, W. W., *Anal. Chem.*, 47, 1528 (1975).
(C20) Dreyer, W. J., Kuppermann, A., Boettger, H. G., Giffin, C. E., Norris, D. D., Grotch, S. L., Theard, L. P., *Clin Chem (Winston-Salem, N.C.)*, 20, 998 (1974).
(C21) Egli, H., Huber, W. K., Seilhofer, H., Vogelsang, R., *Adv. Mass Spectrom.*, 6, 413 (1974).
(C22) Evans, S., Graham, R., *Adv. Mass Spectrom.*, 6, 429 (1974).
(C23) Everdij, J. J., Verster, N. F., *J. Phys. E.*, 8, 603 (1975)
(C24) Fite, W. L., *Int. J. Mass Spectrom. Ion Phys.*, 16, 109 (1975).
(C25) Fite, W. L., Irving, P., *Ind. Res.*, Sept. 1973.
(C26) Ghoshal, S. N., Das, M., Mitra, N. N., *Int. J. Mass Spectrom Ion Phys.*, 17, 67 (1975).
(C27) Gierlich, H. H., Heindrichs, A., Beckey, H. D., *Rev. Sci. Instrum.*, 45, 1208 (1974).
(C28) Giffin, C. E., Boettger, H. G., Norris, D. D., 22nd Annual Conference on Mass Spectrometry and Allied Topics, Philadelphia, Pa., May 1974, p 33.
(C29) Greene, F. T., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, May 1975, p 659.
(C30) Haskins, N. J., Games, D. E., Taylor, K. T., *Biomed. Mass Spectrom.*, 1, 423 (1974).
(C31) Hasted, J. B., *Adv Mass Spectrom.*, 6, 901 (1974)
(C32) Hillenkamp, F., Unsold, E., *Nature (London)*, 256, 119 (1975).
(C33) Hogg, A. M., *Adv. Mass Spectrom.*, 6, 391 (1974).
(C34) Hung, G. W. C., Nunez, L. J., Autian, J., *J. Pharm. Sci.*, 62, 1308 (1973).
(C35) Irako, M., Oguri, T., Kanomata, I., *Jpn. J. Appl Phys.*, 14, 533 (1975).
(C36) King, R. W., Baucom, K. B., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, May 1975, p 651.
(C37) Koslara, A. A., *Optik*, 43, 205 (1975).
(C38) Kruger, V. R., Olander, D. R., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975, p 661.
(C39) Lacey, M. J., Macdonald, C. G., *J. Chem. Soc., Chem. Commun.*, 421 (1975).
(C39A) Lumpkin, H. E., Elliott, R. M., Evans, S., Hazelby, D., Wolstenholme, W. A., Proceedings of the 23rd Conference on Mass Spectrometry and Allied Topics, May 1975, Houston, p 235.
(C40) MacFarlane, R. D., Skowronski, R., Hassell, A., Torgerson, D. F., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975, p 594.
(C41) Magyar, J. J., *Chem. Abstr.*, 83, 747 (1975).
(C42) Maugh, T. H., III, *Science*, 187, 529 (1975).
(C43) Maul, J., Schulz, F., Wittmaack, K., *Adv. Mass Spectrom.*, 6, 493 (1974)
(C44) McEwen, C. N., Bolinski, A. G., *Biomed. Mass Spectrom.*, 2, 112 (1975).
(C45) Means, J. C., Perkins, E. G., *J. Am. Oil Chem. Soc.*, 52, 124A (1975).
(C46) Merritt, C., Jr., Sacher, R. E., Peterson, B. A., *J. Chromatogr.*, 99, 301 (1974).
(C47) Meuzelaar, H. L. C., Kistemaker, P. G., Posthumus, M. A., *Biomed. Mass Spectrom.*, 1, 312 (1974).
(C48) Meyer, E., *Int. J. Mass Spectrom. Ion Phys.*, 13, 123 (1974).
(C49) Miyake, H., Michijima, M., *Adv. Mass Spectrom.*, 6, 529 (1974).
(C50) Myers, R. L., Fite, W. L., *Am. Lab.*, 7(16), 23 (1975).
(C51) Myers, R. L., Fite, W. L., *Environ. Sci. Technol.*, 9, 334 (1975).
(C52) Nakao, F., *Rev. Sci. Instrum.*, 46, 1489 (1975).
(C53) Olson, J. R., Amme, R. C., Keller, G. E., Murcray, D. G., Brooks, J. N., Williamson, P. R., *Bull Am. Phys. Soc., Ser. 2*, 20, 427 (1975).
(C54) Ostrander, L. E., Nelson, A. D., Ernst, E. A., Baetz, W. R., *IEEE Trans. Bio-Med. Eng.*, 22, 448 (1975)
(C55) Quayle, A., *Adv. Mass Spectrom.*, 6, xxiii (1974).
(C56) Rasymakers, J. G. A. M., Engel, D. J. C., *Anal. Chem.*, 46, 1357 (1974)
(C57) Reeher, J. R., Svec, H. J., *Adv Mass Spectrom.*, 6, 509 (1974).
(C58) Richards, J. A., Huey, R. M., Hiller, J., *Int*

*J Mass Spectrom Ion Phys.*, 12, 317 (1973).
(C59) Schoeller, D A., Hayes, J. M., *Anal. Chem.*, 47, 408 (1975)
(C60) Schotzau, H. J., Kneubuhl, F., *IEEE J. Quantum Elec*, QE-11, 81 (1975).
(C61) Simons, D S., Colby, B N., Evans, C. A., Jr., *Int. J. Mass Spectrom. Ion Phys.*, 15, 291 (1974).
(C62) Stavinoha, W. B., Weintraub, S. T., *Anal Chem.*, 46, 757 (1974).
(C63) Torgerson, D. F., Skowronski, R P., MacFarlane, R D., *Biochem. Biophys. Res. Commun.*, 60, 615 (1974).
(C64) Westover, L. B., Tou, J. C., Mark, J. H., *Anal Chem.*, 46, 568 (1974).
(C65) Witiak, J. L., Junk, G. A., Calder, G. V., Fritz, J. S., Svec, H. J., *J. Org. Chem.*, 38, 3066 (1973).
(C66) Wolstenholme, W. A., Elliott, R. M., *Am. Lab.*, 7(11), 68 (1975).
(C67) Wyatt, J. R., DeCorpo, J. J., McDowell, M. V., Saalfeld, F. E., *Adv. Mass Spectrom.*, 6, 541 (1974)
(C68) Wyatt, J. R., DeCorpo, J. J., Saalfeld, F. E., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, May 1975, p 666.

**Chromatographic–Mass Spectrometric–On-Line Computer Techniques**

(D1) Arpino, P., Baldwin, M. A., McLafferty, F. W., *Biomed. Mass Spectrom.*, 1, 80 (1974).
(D2) Arpino, P., Dawkins, B. G., McLafferty, F. W., *J. Chromatogr. Sci.*, 12, 574 (1974).
(D3) Aspinal, M. L., Compson, K. R., Downen, A. A., Elliott, R. M., Hazelby, D., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975, p 73.
(D4) Axelson, M., Cronholm, T., Curstedt, T., Reimendal, R., Sjövall, J., *Chromatographia*, 7, 502 (1974).
(D5) Bell, H. M., *J. Chem. Educ.*, 51, 548 (1974).
(D6) Biller, J. E., Biemann, K., *Anal. Lett.*, 7, 515 (1974).
(D7) Brooks, C. J. W., Middleditch, B. S., in "Mass Spectrometry", Vol. 3, R. A. W. Johnstone, Sr. Reporter, The Chemical Society, Burlington House, London, 1975, p 296.
(D8) Bruner, F., Ciccioli, P., Brancaleoni, E., Longo, A., *Chromatographia*, 8, 503 (1975).
(D9) Burlingame, A. L., Olsen, R. W., McPherron, R., *Adv. Mass Spectrom.*, 6, 1053 (1974).
(D10) Clerc, J. T., Kutter, M., Reinhard, M., Schwarzenbach, R., *J. Chromatogr.*, in press (1976).
(D11) Costa, E., Holmstedt, E., Ed., "Gas Chromatography–Mass Spectrometry in Neurobiology", Advances in Biochemical Psychopharmacology, Vol. 7, Raven Press, New York, 1973.
(D12) Davis, J. E., Shepard, A., Stanford, N., Rogers, L. B., *Anal. Chem.*, 46, 821 (1974).
(D13) (a) Dromey, R. G., Buchanan, B. G., Smith, D. H., Lederberg, J., Djerassi, C., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975, p 486. (b) Dromey, R. G., Buchanan, B. G., Smith, D. H., Lederberg, J., Djerassi, C., *J. Org. Chem.*, 40, 770 (1975).
(D14) Eichelberger, J. W., Harris, L. E., Budde, W. L., *Anal. Chem.*, 47, 995 (1975).
(D15) Eichelberger, J. W., Harris, L. E., Budde, W. L., *Anal. Chem.*, 46, 227 (1974).
(D16) Evans, J. E., Jurinski, N. B., *Anal. Chem.*, 47, 961 (1975).
(D17) Eyem, J., *Chromatographia*, 8, 456 (1975).
(D18) Falkner, F. C., Sweetman, B. J., Watson, J. T., *Appl. Spectrosc. Rev.*, 10, 51 (1975).
(D19) Fenselau, C., *Appl. Spectrosc.*, 28, 305 (1974).
(D20) Fies, W. F., Story, M. S., *Adv. Mass Spectrom.*, 6, 385 (1974).
(D21) Finnigan, R. E., Knight, J. B., Proc. Environmental Chemistry Symposium on Identification and Analysis of Organic Pollutants in Water, Mexico City, Mexico, 1975, in press.
(D22) Flückiger, R., *Chromatographia*, 8, 434 (1975).
(D23) Goedert, M., Wise, S. A., Juvet, R. S., Jr., *Chromatographia*, 7, 539 (1974).
(D24) Hammar, C.-G., Pettersson, G., Carpenter, P. T., *Biomed. Mass Spectrom.*, 1, 397 (1974).
(D25) Hargreaves, R. T., Cook, J. C., Jr., Rinehart, K L., Jr., 22nd Annual Conference on Mass Spectrometry and Allied Topics, Philadelphia, Pa., 1974, p 205.
(D26) Hedfjall, B., Ryhage, R., *Anal. Chem.*, 47, 666 (1975).
(D27) Hedfjäll, B., Ryhage, R., Åkertind, Å., *Adv. Mass. Spectrom.*, 6, 1043 (1974).
(D28) Henneberg, D., Casper, K., Weimann, B., Ziegler, E., *Adv. Mass Spectrom.*, 6, 477 (1974).
(D29) Henneberg, D., Henrichs, U., Schomburg, G., *Chromatographia*, 8, 449 (1975).
(D30) Henneberg, D., Henrichs, U., Schomburg, G., *J. Chromatogr.*, 112, 343 (1975).
(D31) Henneberg, D., Weimann, B., Ziegler, E., *Chromatographia*, 7, 483 (1974).
(D32) Hilmer, R. M., Taylor, J. W., *Anal. Chem.*, 46, 1038 (1974).
(D33) Jones, P. R., Yang, S. K., *Anal. Chem.*, 47, 1000 (1975).
(D34) Justice, J. B., Jr., Isenhour, T. L., *Anal. Chem.*, 47, 2286 (1975).
(D35) Kimble, B J., Cox, R E., McPherron, R. V., Olsen, R. W., Rotman, E., Walls, F. C., Burlingame, A. L., *J. Chromatogr. Sci.*, 12, 647 (1974).
(D36) Kimble, B J., Cox, R E., McPherron, R. V., Olsen, R. W., Rotman, E., Walls, F. C., Burlingame, A. L., 22nd Annual Conference on Mass Spectrometry and Allied Topics, Philadelphia, Pa., 1974, p 315.
(D37) Kimble, B. J., Walls, F. C., Olsen, R. W., Burlingame, A. L., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975, p 503.
(D38) Klein, P D., Haumann, J. R., Hachey, D. L., *Clin. Chem. (Winston-Salem, N.C.)*, 21, 1253 (1975).
(D39) Kushl, D. W., Glass, G. E., Puglisi, F. A., *Anal. Chem.*, 46, 804 (1974).
(D40) Laitinen, H. A., *Anal. Chem.*, 47, 1225 (1975).
(D41) Lee, M. G., Millard, B. J., *Biomed. Mass Spectrom.*, 2, 78 (1975).
(D42) Markey, S. P., Hawks, R. L., Milne, G. W. A., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975, p 197.
(D43) Matthews, D. E., Hayes, J. M., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975, p 482.
(D44) Maurer, D., Archibald, J. A., Rheingold, A. L., *J. Chem. Educ.*, 51, 463 (1974).
(D45) McLafferty, F. W., Dawkins, B. G., *Biochem Soc. Trans.*, 3, 838 (1975).
(D46) McLafferty, F. W., Knutti, R., Venkataraghavan, R., Arpino, P. J., Dawkins, B. G., *Anal. Chem.*, 47, 1503 (1975).
(D47) McPherron, R. V., Burlingame, A. L., *Anal. Chem.*, in preparation.
(D48) Melton, F. A., Mass Spectrom., 3, 117 (1975).
(D49) Merritt, C., Jr., Robertson, D. H., Cavagnaro, J. F., Graham, R. A., Nichols, T. L., *J. Agric. Food Chem.*, 22, 750 (1974).
(D50) Nau, H., Biemann, K., *Anal. Chem.*, 46, 426 (1974).
(D51) Neuner-Jehle, N., Etzweiler, F., Zarske, G., *Chromatographia*, 7, 323 (1974).
(D52) Palmer, L., Holmstedt, B., *Sci. Tools*, 22, 1215 (1975).
(D53) Parsles, S. R., Rosen, J. D., *Anal Chem.*, 47, 1215 (1975).
(D54) Rapp, U., Schröder, U., Meier, S., Elmenhorst, H., *Chromatographia*, 8, 474 (1975).
(D55) Richter, W. J., Blum, W., Liehr, J. G., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975, p 591; Blum, W., Schlumpf, E., Liehr, J. G., Richter, W. J., *Tetrahedron Lett.*, 7, 565 (1976).
(D56) Rozett, R. W., *Anal. Chem.*, 46, 2085 (1974).
(D57) Rozett, R. W., Petersen, E. M., *Anal. Chem.*, 47, 1301 (1975).
(D58) Scott, R. P. W., Scott, C. G., Munroe, M., Hess, J., Jr., *J. Chromatogr.*, 99, 395 (1974).
(D59) Strong, J. M., Atkinson, A. J., Jr., Ferguson, R. J., *Anal. Chem.*, 47, 1720 (1975).
(D60) Sweeley, C. C., Young, N. D., Holland, J. F., Gates, S. C., *J. Chromatogr.*, 99, 507 (1974).
(D61) Thomas, B. R., *J. Chromatogr.*, 109, 168 (1975).
(D62) van't Klooster, H. A., Vaarkamp-Lijnse, J. S., Dijkstra, G., *Org. Mass Spectrom.*, 8, 303 (1974).
(D63) Wolen, R. L., Pierson, H. E., *Anal. Chem.*, 47, 2068 (1975).
(D64) Young, N. D., Holland, J. F., Gerber, J. N., Sweeley, C. C., *Anal. Chem.*, 47, 2373 (1975).

**Mass Spectral Management and Interpretation Techniques**

(E1) Abe, H., Jurs, P. C., *Anal. Chem.*, 47, 1829 (1975).
(E2) Abramson, F. P., *Anal Chem.*, 47, 45 (1975).
(E3) Brodskii, E. S., *J. Anal Chem. USSR*, 29, 476 (1974).
(E4) Carhart, R. E., Smith, D E., Brown, H., Djerassi, C., *J. Am. Chem Soc.*, 97, 5755 (1975)
(E5) Clerc, T., Erni, F., *Top. Curr Chem.*, 39, 91 (1973)
(E6) Dayringer, H. E., Pesyna, G M., Venkataraghavan, R., McLafferty, F. W., *Org Mass Spectrom.*, in press.
(E7) Delfino, A. B., Buchs, A., *Top. Curr Chem.*, 39, 110 (1973).
(E8) Dromey, R G., Buchanan, B. G., Smith, D. H., Lederberg, J., Djerassi, C., *J. Org Chem.*, 40, 770 (1975).
(E9) Franzen, J., *Chromatographia*, 7, 518 (1974).
(E10) Gray, N. A. B., *Adv. Mass Spectrom.*, 6, 1073 (1974).
(E11) Gray, N. A. B., *Org. Mass Spectrom.*, 10, 507 (1975)
(E12) Gray, N. A. B., Grönneberg, T. Ö., *Anal. Chem.*, 47, 419 (1975).
(E13) Gray, N. A. B., Zoro, J. A., Grønneberg, T. O., Gaskell, S. J., Cardoso, J. N., Eglinton, G., *Anal. Lett.*, 8, 461 (1975).
(E14) Gronneberg, T. Ö., Gray, N. A. B., Eglinton, G., *Anal. Chem.*, 47, 415 (1975).
(E15) Grotch, S. L., 22nd Annual Conference on Mass Spectrometry and Allied Topics, Philadelphia, Pa., 1974, p 456.
(E15A) Grotch, S. L., *Anal Chem.*, 47, 1285 (1975)
(E16) Heller, S. R., Chang, C. L., Chu, K. C., *Anal. Chem.*, 46, 951 (1974).
(E17) Heller, S. R., Fales, H. M., Milne, G. W. A., Feldmann, R. J., Daly, N. R., Maxwell, D. C., McCormick, A., *Adv. Mass. Spectrom.*, 6, 1037 (1974).
(E18) Heller, S. R., Fales, H M., Milne, G. W. A., Heller, R. S., McCormick, A., Maxwell, D. C., *Biomed. Mass Spectrom.*, 1, 207 (1974).
(E19) Heller, S. R., Koniver, D. A., Fales, H. M., Milne, G. W. A., *Anal. Chem.*, 46, 947 (1974).
(E20) Isenhour, T. L., Justice, J. B., *Adv. Mass Spectrom.*, 6, 981 (1974).
(E21) Isenhour, T. L., Kowalski, B. R., Jurs, P. C., *Crit. Rev. Anal. Chem.*, 4, 1 (1974).
(E22) Kent, P., Gaumann, T., *Helv. Chim. Acta*, 58, 787 (1975).
(E23) Legeot, C., *J. Organomet. Chem.*, 98, 355 (1975).
(E24) Masinter, L. M., Sridharan, N. S., Carhart, R. E., Smith, D. H., *J. Am. Chem. Soc.*, 96, 7714 (1974).
(E25) Mathews, R. J., *Aust. J. Chem.*, 28, 1955 (1973).
(E26) Mathews, R. J., *Int. J. Mass Spectrom. Ion Phys.*, 17, 217 (1975).
(E27) Mathews, R. J., Morrison, J. D., *Aust. J. Chem.*, 27, 2167 (1974).
(E28) McLafferty, F. W., Dayringer, H. E., Venkataraghavan, R., *Ind. Res.*, 16, 78 (1976).
(E29) McLafferty, F. W., Hertel, R. H., Villwock, R. D., *Org. Mass Spectrom.*, 9, 690 (1974).
(E30) McLafferty, F. W., Venkataraghavan, R., Kwok, K.-S., Pesyna, G., *Adv. Mass Spectrom.*, 6, 999 (1974).
(E30A) Pesyna, G. M., McLafferty, F. W., Venkataraghavan, R., Dayringer, H. E., *Anal. Chem.*, 47, 1161 (1975).
(E31) Pesyna, G. M., Venkataraghavan, R., Dayringer, H. E., McLafferty, F. W., *Anal. Chem.*, submitted.
(E32) Ritter, G. L., Lowry, S. R., Wilkins, C. L., Isenhour, T. L., *Anal. Chem.*, 47, 1951 (1975).
(E33) Robertson, D. H., Merritt, C., Jr., 21st Annual Conference on Mass Spectrometry and Allied Topics, San Francisco, Calif., 1973, p 65.
(E34) Smith, D. H., *Anal. Chem.*, 47, 1178 (1975).
(E35) Smith, J. F., Mathews, R. J., Morrison, J. D., 23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975, p 493.
(E36) Stonham, T. J., Aleksander, I., Camp, M., Pike, W. T., Shaw, M. A., *Anal. Chem.*, 47, 1817 (1975).
(E37) Venkataraghavan, R., Kwok, K.-S., Pesyna, G., McLafferty, F. W., 21st Annual Conference on Mass Spectrometry and Allied Topics, San Francisco, Calif., 1973, p 197.
(E38) Vink, J., Heerma, W., Kamerling, J. P., Vliegenthart, J. F. G., *Org. Mass Spectrom.*, 9, 536 (1974).
(E39) Zander, G. S., Jurs, P. C., *Anal. Chem.*, 47, 1562 (1975).

**Electron Impact and Organic Mass Spectrometry**

(F1) Acheson, R. M., Aplin, R T., Bolton, R. G., *Org. Mass Spectrom.*, 8, 95 (1974)
(F2) Aldous, G. L., Bowie, J. H., *Org. Mass Spectrom.*, 10, 64 (1975).

(F3) Baldwin, M. A., McLafferty, F. W., Jerina, D. M., *J. Am Chem Soc.*, 97, 6169 (1975)
(F4) Block, J. H., Smith, D. H., Djerassi, C., *J. Org Chem*, 39 279 (1974)
(F5) Bosshardt, H., Hesse, M., *Angew. Chem., Int. Ed. Engl.*, 13, 252 (1974).
(F6) Budzikiewicz, H., Lenz, U., *Org. Mass Spectrom*, 10, 987 (1975).
(F7) Derrick, P. J., Falick, A. M., Burlingame, A. L., *J. Chem. Soc., Perkin Trans. 2*, 981 (1975).
(F8) Dougherty, R. C., "Dynamic Chemistry", *Top Curr Chem.*, 45, 93 (1974).
(F9) Eadon, G., Gold, P., Bacon, E., *J. Am. Chem. Soc*, 97, 5184 (1975).
(F10) Eggelte, T. A., Nibbering, N. M. M., *J. Chem. Soc., Perkin Trans. 2*, 605 (1974).
(F11) Fetizon, M., Henry, Y., Aranda, G., Audier, H. E., de Luzer, H., *Org. Mass Spectrom.*, 8, 201 (1974).
(F12) Fiaux, A., Wirz, B., Gäumann, T., *Helv. Chim. Acta*, 57, 525 (1974).
(F13) Fitch, W. L., Djerassi, C., *J. Am. Chem. Soc.*, 96, 4917 (1974).
(F14) Gray, R. T., *Org. Mass Spectrom.*, 9, 346 (1974).
(F15) Green, M. M., Moldowan, J. M., McGrew, J. G., *J. Org. Chem.*, 39, 2166 (1974).
(F16) Grigsby, R. D., Jamieson, W. D., McInnes, A. G., Maass, W. S. G., Taylor, A., *Can. J. Chem.*, 52, 4117 (1974).
(F17) Gusten, H., Klasinc, L., Kramer, V., Marsel, J., *Org. Mass Spectrom.*, 8, 323 (1974).
(F18) Hansen, P. E., Undheim, K., *Acta Chem. Scand., Ser. B*, 29, 221 (1975).
(F19) Heitke, B. T., McCarty, C. G., *Can. J. Chem.*, 52, 2861 (1974).
(F20) Henion, J. D., Kingston, D. G. I., *J. Am. Chem Soc.*, 96, 2532 (1974).
(F21) Hittenhausen-Gelderblom, R., Venema, A., Nibbering, N. M. M., *Org. Mass Spectrom.*, 9, 878 (1974).
(F22) Ito, T. I., Weber, W. P., *J. Org. Chem.*, 39, 1691 (1974).
(F23) Jackson, W. M., Brackmar, R. T., Fite, W. L., *Int. J. Mass Spectrom. Ion Phys.*, 12, 237 (1974).
(F24) Jaeger, D. A., Tomer, K. B., Woodgate, P. D., Gebreyesus, T., Djerassi, C., Shapiro, R. H., *Org. Mass Spectrom.*, 9, 551 (1974).
(F25) Jauregu, J. F., Lehmann F., P.A., *Org. Mass Spectrom.*, 9, 58 (1974).
(F26) King, G. S., Waight, E. S., *J. Chem. Soc., Perkin Trans. 1*, 1499 (1974).
(F27) Kingston, D. G. I., Tannenbaum, H. P., *Org. Mass Spectrom.*, 10, 263 (1975).
(F28) Kingston, D. G. I., Bursey, J. T., Bursey, M. M., *Chem. Rev.*, 74, 215 (1974).
(F29) Köppel, C., Schwarz, H., Bohlmann, F., *Org. Mass Spectrom.*, 9, 343 (1974).
(F30) Leduc, G., Rousseau, Y., *Can. J. Chem.*, 52, 1648 (1974).
(F31) Lin, D. C. K., De Jongh, D. C., *J. Org. Chem.*, 39, 1780 (1974).
(F32) Lin, D. C. K., Thomson, M. L., De Jongh, D. C., *Can. J. Chem.*, 52, 2359 (1974).
(F33) Lin, M. S.-H., Harrison, A. G., *Can. J. Chem.*, 52, 1813 (1974).
(F34) Longevialle, P., Alazard, J. P., Lusinchi, X., *Org. Mass Spectrom.*, 9, 480 (1974).
(F35) Maquestiau, A., van Haverbeke, Y., Flammang, R., Cooks, R. G., *Org. Mass Spectrom.*, 10, 946 (1975).
(F36) Maquestiau, A., van Haverbeke, Y., de Meyer, C., Flammang, R., *Org. Mass Spectrom.*, 9, 149 (1974).
(F37) Maquestiau, A., van Haverbeke, Y., de Meyer, C., Katritzky, A. R., Cook, M. J., Page, A. D., *Can J. Chem*, 53, 490 (1975).
(F38) Meyerson, S., Karabatsos, G. J., *Org. Mass Spectrom.*, 8, 289 (1974).
(F39) Meyerson, S., Fields, E. K., *Org. Mass Spectrom.*, 9, 485 (1974).
(F40) Molenaar-Langeveld, T. A., Nibbering, N. M. M., *Org. Mass Spectrom.*, 9, 257 (1974).
(F41) Muccino, R. R., Djerassi, C., *J. Am. Chem. Soc.*, 96, 556 (1974).
(F42) Rebane, E., *Chem Scr.*, 5, 5 (1974).
(F43) Rebane, E., *Chem. Scr.*, 5, 65 (1974).
(F44) Rebane, E., *Chem Scr.*, 4, 219 (1973).
(F45) Resink, J. J., Venema, A., Nibbering, N. M. M., *Org. Mass Spectrom.*, 9, 1055 (1974)
(F46) Schoemaker, H. E., Nibbering, N. M. M., Cooks, R. G., *J. Am Chem Soc.*, 97, 4415 (1975).
(F47) Schwarz, H., *Org. Mass Spectrom.*, 10, 384 (1975)
(F48) Siegel, A., *J. Am. Chem. Soc.*, 96, 1251 (1974).
(F49) Tajima, S., Tsuchiya, T., *Org. Mass Spectrom.*, 9, 265 (1974).
(F50) Thomson, M. L., De Jongh, D. C., *Can. J. Chem*, 51, 3313 (1973)
(F51) Tomer, K. B., *Org. Mass Spectrom.*, 10, 480 (1975)
(F52) Tomer, K. B., Djerassi, C., *Tetrahedron*, 30, 17 (1974)
(F53) Tsuchiya, M., Adachi, Y., *Int. J Mass Spectrom. Ion Phys.*, 19, 222 (1975)
(F54) van den Heuvel, C. G., Nibbering, N. M. M., *Org Mass Spectrom*, 10, 250 (1975)
(F55) Van de Sande, C. C., McLafferty, F. W., *Org. Mass Spectrom.*, 10, 561 (1975)
(F56) Venema, A., Nibbering, N. M. M., *Org. Mass Spectrom.*, 9, 1234 (1974).
(F57) Venema, A., Nibbering, N. M. M., *Org. Mass Spectrom.*, 9, 628 (1974).
(F58) von Minden, D. L., Liehr, J. G., Wilson, M. H., McCloskey, J. A., *J. Org. Chem.*, 39, 285 (1974).
(F59) Weinstein, S., Gil-Av, E., Leftin, J. H., Levy, E. C., Mandelbaum, A., *Org. Mass Spectrom.*, 9, 774 (1974).
(F60) Whitfield, G. F., Beilan, H. S., Saika, D., Sivern, D., *J. Org. Chem.*, 39, 2148 (1974).
(F61) Winnik, M. A., Saunders, D., Jackowski, G., Trueman, R. E., *J. Am. Chem. Soc.*, 96, 7510 (1974).

### Field Ionization Kinetics

(G1) Baldwin, M. A., Derrick, P. J., Morgan, R. P., *Int. J. Mass Spectrom. Ion Phys.*, in press (1976).
(G2) Derrick, P. J., in "Mass Spectrometry", A. Maccoll, Ed., *Int. Rev. Sci., Physical Chemistry Ser. Two*, Vol 5, Butterworths, London and Boston, Mass., 1975, p. 1.
(G3) Derrick, P. J., Burlingame, A. L., *Acc. Chem. Res.*, 7, 328 (1974).
(G4) Derrick, P. J., Burlingame, A. L., *J. Am. Chem. Soc.*, 96, 4909 (1974).
(G5) Derrick, P. J., Falick, A. M., Burlingame, A. L., *Adv. Mass Spectrom.*, 6, 877 (1974).
(G6) Derrick, P. J., Falick, A. M., Burlingame, A. L., *J. Am. Chem. Soc.*, 96, 615 (1974).
(G7) Derrick, P. J., Falick, A. M., Burlingame, A. L., *J. Chem. Soc. Faraday Trans 1*, 71, 1503 (1975).
(G8) Derrick, P. J., Falick, A. M., Burlingame, A. L., Djerassi, C., *J. Am. Chem. Soc.*, 96, 1054 (1974).
(G9) Derrick, P. J., Holmes, J. L., Morgan, R. P., *J. Am. Chem. Soc.*, 97, 4936 (1975).
(G10) Derrick, P. J., Morgan, R. P., Hill, J. T., Baldwin, M. A., *Int. J. Mass Spectrom. Ion Phys.*, 18, 393 (1975).
(G11) Falick, A. M., Burlingame, A. L., *J. Am. Chem. Soc.*, 97, 1525 (1975).
(G12) Hirsch, R. G., Van Brunt, R. J., Whitehead, W. D., *Int. J. Mass Spectrom. Ion Phys.*, 17, 335 (1975).
(G13) Lehmann, W. D., Beckey, H. D., *Org. Mass Spectrom.*, 9, 1086 (1974).
(G14) Levsen, K., Beckey, H. D., *Int. J. Mass Spectrom. Ion Phys.*, 14, 45 (1974).
(G15) Levsen, K., Beckey, H. D., *Int. J. Mass Spectrom. Ion Phys.*, 15, 333 (1974).
(G16) Levsen, K., Beckey, H. D., *Int. J. Mass Spectrom. Ion Phys.*, 15, 353 (1974).
(G17) Morgan, R. P., Derrick, P. J., *J. Chem. Soc., Chem. Commun.*, 836 (1974).
(G18) Morgan, R. P., Derrick, P. J., *Org. Mass Spectrom.*, 10, 563 (1975).
(G19) Smith, R. D., Futrell, J. H., *Int. J. Mass Spectrom. Ion Phys.*, 17, 233 (1975).

### Appearance Potentials

(H1) Baer, T., Werner, A. S., Tsai, B. P., Lin, S. F., *J. Chem. Phys.*, 61, 5468 (1974).
(H2) Benoit, F. M., *Org. Mass Spectrom.*, 9, 626 (1974).
(H3) Beynon, J. H., Cooks, R. G., Jennings, K. R., Ferrer-Correia, A. J., *Int. J. Mass Spectrom. Ion Phys.*, 18, 87 (1975).
(H4) Buttrill, S. E., Magil, G. C., *Int. J. Mass Spectrom. Ion Phys.*, 17, 287 (1975).
(H5) Buttrill, S. E., Williamson, A. D., LeBreton, P., *J. Chem Phys.*, 62, 1586 (1975).
(H6) Carbonneau, R., Marmet, P., *Phys. Rev. A*, 9, 1898 (1974).
(H7) Conrath, K., Van de Sande, C., Vandewalle, M., *Org. Mass Spectrom.*, 9, 585 (1974).
(H8) Coppens, P., Smets, J., Fishel, M. G., Drowart, J., *Int. J. Mass Spectrom. Ion Phys.*, 14, 57 (1974).
(H9) Dromey, R. G., Morrison, J. D., Traeger, J. C., *Int. J. Mass Spectrom. Ion Phys.*, 6, 57 (1971)
(H10) Finney, C. D., Sung, J. P., Finney, K. A., *Int. J Mass Spectrom. Ion Phys.*, 13, 459 (1974).
(H11) Gordon, S. M., Reid, N. W., *Int. J. Mass Spectrom. Ion Phys.*, 18, 379 (1975).
(H12) Green, M. M., Bayfus, D., Franklin, J. L., *Org Mass Spectrom*, 10, 679 (1975).
(H13) Gross, M. L., Wilkins, C. L., Williams, R. C., Leung, G., *Org Mass Spectrom.*, 9, 1217 (1974).
(H14) Heller, R., Varmuza, K., Krenmayr, P., *Monatsh Chem*, 105, 787 (1974)
(H15) Holmes, J. L., *Org. Mass Spectrom.*, 8, 247 (1974)
(H16) Hubin-Franskin, M. J., Hemesch, J., Collin, J. E., *Int. J. Mass Spectrom. Ion Phys.*, 13, 131 (1974).
(H17) Johnson, L. P., Morrison, J. D., *Int. J. Mass Spectrom. Ion Phys.*, 18, 355 (1975).
(H18) Johnstone, R. A. W., McMaster, B. N., *Adv. Mass Spectrom.*, 6, 451 (1974).
(H19) Knowles, D. J., Nicholson, A. J. C., *J. Chem Phys.*, 60, 1180 (1974).
(H20) Koenig, T., Balle, T., Snell, W., *J. Am Chem Soc.*, 97, 662 (1975).
(H21) Kollman, K., *Int. J. Mass Spectrom. Ion Phys.*, 17, 261 (1975).
(H22) Koppel, C., Schwarz, H., Bohlmann, F., *Org. Mass Spectrom.*, 8, 25 (1974).
(H23) Lifshitz, C., Mackenzie-Peers, A., Weiss, M., Weiss, M. J., *Adv. Mass Spectrom.*, 6, 871 (1974)
(H24) Lossing, F. P., Traeger, J. C., *J. Am. Chem. Soc.*, 97, 1579 (1975).
(H25) Loudon, A. G., Mazengo, R. Z., *Org. Mass Spectrom.*, 8, 179 (1974).
(H26) Maeda, K., Suzuki, I. H., Kayama, Y., *Int. J. Mass Spectrom. Ion Phys.*, 14, 273 (1974).
(H27) McCulloh, K. E., Walker, J. A., *Chem. Phys. Lett.*, 25, 439 (1974).
(H28) Occolowitz, J. L., Cerimele, B. J., Brown, P., *Org. Mass Spectrom.*, 8, 61 (1974).
(H29) Richards, K. E., McMaster, B. N., Wright, G. J., *Org Mass Spectrom.*, 10, 295 (1975).
(H30) Schowengerdt, F. D., Golden, D. E., *Rev. Sci. Instrum.*, 45, 391 (1974).
(H31) Solka, B. H., Russell, M. E., *J. Phys. Chem.*, 78, 1268 (1974).
(H32) Suzuki, I. H., Maeda, K., *Int. J. Mass Spectrom. Ion Phys.*, 13, 293 (1974).
(H33) Suzuki, I. H., Maeda, K., *Int. J. Mass Spectrom. Ion Phys.*, 18, 261 (1974).
(H34) Werner, A. S., Tsai, B. P., Baer, T., *J. Chem. Phys.*, 60, 3650 (1974).

### Translational Energy Release and Metastables

(I1) Baldwin, M. A., Derrick, P. J., Morgan, R. P., *Org. Mass Spectrom.*, 11, in press (1976).
(I2) Bente, P. F., III, McLafferty, F. W., McAdoo, D. J., Lifshitz, C., *J. Phys. Chem.*, 79, 713 (1975).
(I3) Beynon, J. H., Brothers, D. F., Cooks, R. G., *Anal. Chem.*, 46, 1299 (1974).
(I4) Beynon, J. H., Caprioli, R. M., Cooks, R. G., *Org. Mass Spectrom.*, 9, 1 (1974).
(I5) Brady, L. G., Williams, D. H., Traynor, S. C., Crowley, K. J., *Org. Mass Spectrom.*, 10, 116 (1975).
(I6) Compernolle, F., De Schryver, F., *J. Am. Chem. Soc.*, 97, 3909 (1975).
(I7) Cooks, R. G., Kim, K. C., Beynon, J. H., *Chem. Phys. Lett.*, 26, 131 (1974).
(I8) Cooks, R. G., Kim, K. C., Beynon, J. H., *Int. J. Mass Spectrom. Ion Phys.*, 18, 245 (1974).
(I9) Cooks, R. G., Terwilliger, D. T., Beynon, J. H., *J. Chem. Phys.*, 61, 1208 (1974).
(I10) Curn, G., Romeo, G., Uccella, N., *Org. Mass Spectrom.*, 9, 365 (1974).
(I11) Elder, J. F., Beynon, J. H., Cooks, R. G., *Org. Mass Spectrom.*, 10, 273 (1975).
(I12) Falick, A. M., Tecon, P., Gaumann, T., *Org. Mass Spectrom.*, in press (1976).
(I13) Gordon, S. M., Krige, G. J., Reid, N. W., *Int. J. Mass Spectrom. Ion Phys.*, 14, 109 (1974).
(I14) Holmes, J. L., *Org. Mass Spectrom.*, 8, 247 (1974).
(I15) Holmes, J. L., McGillivray, D., Isaacs, N. S., *Org. Mass Spectrom*, 9, 510 (1974).
(I16) Holmes, J. L., Terlouw, J. K., *Can. J. Chem.*, 53, 2076 (1975).
(I17) Holmes, J. L., Terlouw, J. K., *Org. Mass Spectrom*, 10, 787 (1975).
(I18) Holmes, J. L., Weese, G. M., *Org. Mass Spectrom*, 9, 618 (1974).
(I19) Holzmann, V. G., Minkwitz, R., *Z. Anorg. Allg. Chem.*, 413, 72 (1975).
(I20) Howe, I., *Org. Mass Spectrom.*, 10, 767 (1975).
(I21) Hvistendahl, G., Williams, D. H., *J. Chem. Soc., Chem Commun.*, 4 (1975).

(I22) Hvistendahl, G., William, D. H., *J Am. Chem. Soc.*, 97, 3097 (1975)
(I23) Keough, T., Beynon, J. H., Cooks, R G., Chang, C., Shapiro, R. H., *Z. Naturforsch. A*, 29, 507 (1974).
(I24) Keyes, B. G., Harrison, A. G., *Org. Mass Spectrom.*, 9, 221 (1974).
(I25) Kim, K. C., Beynon, J. H , Cooks, R. G., *J. Chem. Phys.*, 61, 1305 (1974).
(I26) Kim, K. C., Cooks, R. G., *J. Org Chem.*, 40, 511 (1975)
(I27) Krenmayr, P , *Monatsch. Chem* , 106, 925 (1975).
(I28) Lau, A. Y-K, Solka, B. H , Harrison, A. G., *Org. Mass. Spectrom.*, 9, 555 (1974)
(I29) Levin, G., Platzner, I., *J. Chem. Phys.*, 60, 2007 (1974)
(I30) Maslen, V. W., *Int. J. Mass Spectrom. Ion Phys.*, 13, 207 (1974).
(I31) McAdoo, D. J., Bente, P. F., III, Gross, M. L., McLafferty, F W., *Org. Mass Spectrom.*, 9, 525 (1974).
(I32) Meier, K., Seibl, J., *Int. J. Mass Spectrom. Ion Phys.*, 14, 99 (1974).
(I33) Pritchard, J. G., *Org. Mass Spectrom.*, 8, 103 (1974).
(I34) Safe, S., Jamieson, W. D., Embree, D. J., *Can. J. Chem.*, 52, 867 (1974).
(I35) Schlunegger, U. P., *Angew. Chem., Int. Ed. Engl.*, 14, 679 (1975).
(I36) Sen Sharma, D. K., Franklin, J. L., *Int. J. Mass Spectrom. Ion Phys.*, 13, 139 (1974).
(I37) Smith, D . H., Djerassi, C., Maurer, K., Rapp, U., *J. Am Chem. Soc.*, 96, 3482 (1974).
(I38) Solka, B. H., Beynon, J. H., Cooks, R. G., *J. Phys Chem.*, 79, 859 (1975)
(I39) Stefanovic, D., Stambolija, L., *Ann. Chim. (Rome)*, 64, 207 (1974).
(I40) Terwilliger, D. T., Cooks, R. G., Beynon, J. H., *Int. J. Mass Spectrom. Ion Phys.*, 18, 43 (1975).
(I41) Terwilliger, D. T., Beynon, J. H., Cooks, R. G., *Int. J. Mass Spectrom. Ion Phys.*, 14, 15 (1974).
(I42) Terwilliger, D. T., Beynon, J. H., Cooks, R. G., *Proc. Roy. Soc. London, Ser A*, 341, 135 (1974).
(I43) Terwilliger, D. T., Elder, J. F., Beynon, J. H., Cooks, R. G., *Int. J. Mass Spectrom. Ion Phys.*, 16, 225 (1975).
(I44) Uccella, N., *Org. Mass Spectrom.*, 10, 494 (1975).
(I45) Venema, A., Nibbering, N. M. M., Maurer, K. H., Rapp, U., *Int. J. Mass Spectrom. Ion Phys.*, 17, 89 (1975).
(I46) Vijfhuizen, P. C., Heerma, W., Dijkstra, G., *Org. Mass Spectrom.*, 10, 919 (1975).
(I47) Williams, D. H., Hvistendahl, G., *J. Am. Chem. Soc.*, 96, 6753 (1974).
(I48) Williams, D. H., Hvistendahl, G., *J. Am. Chem. Soc.*, 96, 6755 (1974).

### Photoionization

(J1) Ajello, J. M., Huntress, W. T., Lane, A. L., LeBreton, P. R., Williamson, A. D., *J. Chem. Phys.*, 60, 1211 (1974).
(J2) Ajello, J. M., Rayermann, P., *J. Chem. Phys.*, 62, 2917 (1975).
(J3) Akhtar, Z. M., Brion, C. E., Hall, L. D., *Org. Mass Spectrom.*, 8, 189 (1974).
(J4) Baer, T., Werner, A. S., Tsai, B. P., *J. Chem. Phys.*, 62, 2497 (1975).
(J5) Bloch, M., Turner, D. W., *Chem. Phys. Lett.*, 30, 344 (1975).
(J6) Brehm, B., Frey, R., Kustler, A., Eland, J. H. D., *Int. J. Mass Spectrom. Ion Phys.*, 13, 251 (1974).
(J7) Buttrill, S. E., Jr., *J. Chem. Phys.*, 61, 619 (1974).
(J8) Buttrill, S. E., Jr., *J. Chem. Phys.*, 62, 1603 (1975).
(J9) Buttrill, S. E., Jr., *J. Chem. Phys.*, 62, 1834 (1975).
(J10) Buttrill, S. E., Jr., Kim, J. K., Huntress, W. T., Jr., LeBreton, P., Williamson, A., *J. Chem Phys.*, 61, 2122 (1974).
(J11) Collin, G. J., Ausloos, P., *Can. J. Chem.*, 53, 680 (1975).
(J12) Dehmer, P. M., Chupka, W. A., *J. Chem. Phys.*, 62, 2228 (1975).
(J13) Dehmer, P. M., Chupka, W. A., *J. Chem. Phys.*, 62, 4525 (1975).
(J14) Eland, J. H. D., *Int. J. Mass Spectrom. Ion Phys.*, 13, 457 (1974).
(J15) Eland, J. H. D., Schulte, H., *J. Chem. Phys.*, 62, 3835 (1975).
(J16) Foster, M S., Williamson, A. D., Beauchamp, J. L., *Int. J. Mass Spectrom. Ion Phys.*, 18, 429 (1974).
(J17) Gant, C S. T , Danby, C. J , Eland, J. H D., *J. Chem Soc., Faraday Trans. 2*, 71, 1015 (1975).
(J18) Judge, D. L., Lee, L C., *Int J. Mass Spectrom Ion Phys.*, 17, 329 (1975).
(J19) Lifshitz, C., *J. Chem. Phys.*, 62, 1602 (1975).
(J20) Orlov, V. M., Varshavsky, Ya. M., Miroshnikov, A I., *Org. Mass Spectrom.*, 9, 801 (1974).
(J21) Orlov, V. M., Varshavsky, Ya. M., Miroshnikov, A I., *Org. Mass Spectrom.*, 9, 811 (1974).
(J22) Parr, G R., Taylor, J. W , *Int. J. Mass Spectrom Ion Phys.* 14, 467 (1974)
(J23) Simm, I. G., Danby, C. J., Eland, J. H. D., *Int. J. Mass Spectrom. Ion Phys.*, 14, 285 (1974).
(J24) Stockbauer, R., Inghram, M. G., *J. Chem. Phys.*, 62, 4862 (1975).
(J25) Tanaka, K., Honma, K., Koyaro, I., Tanaka, I., *J Chem. Phys.*, 60, 3347 (1974).
(J26) Tsai, B., Baer, T., Horovitz, M. L., *Rev. Sci. Instrum.*, 45, 494 (1974).
(J27) Tsai, B. P., Werner, A. S., Baer, T., *J. Chem. Phys.*, 63, 4384 (1975)
(J28) Tsai, B. P., Werner, A. S., Baer, T., *J. Chem. Phys.*, accepted Aug. 7, 1975.
(J29) Tsai, B. P., Werner, A. S., Lin, S. F., *J. Phys. Chem.*, 79, 570 (1975).
(J30) Turner, D. L., Bone, L. I., *J. Phys. Chem.*, 78, 501 (1974).
(J31) Wei, L. Y., Bone, L. I., *J. Phys. Chem.*, 78, 2527 (1974).
(J32) Werner, A. S., Baer, T., *J. Chem. Phys.*, 62, 2900 (1975).
(J33) Wincel, H., Herman, J. A., *Int. J. Mass Spectrom. Ion Phys.*, 14, 139 (1974).

### Unimolecular Rate Theory

(K1) Alexandru, G., *Int. J. Mass Spectrom. Ion Phys.*, 13, 313 (1974).
(K2) Guttman, C., Rice, S. A., *J. Chem. Phys.*, 61, 651 (1974).
(K3) Hansen, D. A., Lee, E. K. C., *J. Chem. Phys.*, 62, 183 (1975).
(K4) Huang, C.-S., Lin, E. C., *J. Chem. Phys.*, 62, 3826 (1975).
(K5) Hui, M. H., Rice, S. A., *J. Chem. Phys.*, 61, 833 (1974).
(K6) Kanamaru, N., Lin, E. C., *J. Chem. Phys.*, 62, 3252 (1975).
(K7) Levine, R. D., *Ber. Bunsenges. Phys. Chem.*, 78, 111 (1974).
(K8) Meagher, J. F., Chao, K. J., Barker, J. R., Rabinovitch, B. S., *J. Phys. Chem.*, 78, 2535 (1974).
(K9) Nordholm, K. S. J., Rice, S. A., *J. Chem. Phys.*, 61, 203 (1974).
(K10) Nordholm, S., Rice, S. A., *J. Chem. Phys.*, 62, 157 (1975).
(K11) Poclus, A. V., Yardley, J. T., *J. Chem. Phys.*, 61, 2779 (1974).
(K12) Rabinovitch, B. S., Meagher, J. F., Chao, K.-J., Barker, J. R., *J. Chem. Phys.*, 60, 2932 (1974).
(K13) Stein, S. E., Rabinovitch, B. S., *J. Chem. Phys.*, 60, 908 (1974).
(K14) Thayer, C. A., Poclus, A. V., Yardley, J. T., *J. Chem. Phys.*, 62, 3712 (1975).
(K15) Thayer, C. A., Yardley, J. T., *J. Chem. Phys.*, 61, 2487 (1974).

### Molecular Orbital Calculations

(L1) Bernardi, F., Calzmadia, I. G., Schlegel, H. B., Wolfe, S., *Can. J. Chem.*, 53, 1144 (1975).
(L2) Bischof, P. K., Dewar, M. J. S., *J. Am. Chem. Soc.*, 97, 2278 (1975).
(L3) Bursey, M. M., Kao, J.-L., Pedersen, L., *Org. Mass Spectrom.*, 10, 38 (1975).
(L4) Chu, S. Y., Goodman, L., *J. Am. Chem. Soc.*, 97, 7 (1975).
(L5) Cremaschi, P., Simonetta, M., *Theor. Chim. Acta*, 34, 175 (1974).
(L6) Calzmadia, I. G., Duke, A. J., Lucchini, V., Modena, G., *J. Chem. Soc., Perkin Trans. 2*, 1808 (1974).
(L7) Calzmadia, I. G., Lucchini, V., Modena, G., *Theor. Chim. Acta*, 39, 51 (1975).
(L8) Davis, T. D., Maggiora, G. M., Christoffersen, R. E., *J. Am. Chem. Soc.*, 96, 7878 (1974).
(L9) Devaquet, A. J. P., Hehre, W. J., *J. Am. Chem. Soc.*, 96, 3644 (1974).
(L10) Dewar, M. J. S., *J. Am. Chem. Soc.*, 96, 5240 (1974).
(L11) Dewar, M. J. S., *J. Am. Chem. Soc.*, 97, 6591 (1975).
(L12) Dyczmons, V., Kutzelnigg, W., *Theor. Chem Acta*, 33, 239 (1974).
(L13) Gallup, G. A., Nabeck, J. M., *J. Am. Chem. Soc.*, 97, 970 (1975).
(L14) Hariharan, P C., Radom, L., Pople, J. A., Schleyer, P. v. R., *J. Am. Chem. Soc.*, 96, 599 (1974).
(L15) Hay, P. J., Shavitt, I., *J. Chem. Phys.*, 60, 2865 (1974).
(L16) Hehre, W J., *Acc. Chem. Res.*, 8, 369 (1975).
(L17) Hehre, W J., *J. Am. Chem. Soc.*, 96, 5207 (1974).
(L18) Hehre, W J., *J Am. Chem. Soc.*, 97, 5308 (1975).
(L19) Hehre, W J., Hiberty, P. C., *J. Am. Chem. Soc.*, 96, 302 (1974)
(L20) Hehre, W. J., Hiberty, P. C., *J. Am. Chem. Soc.*, 96, 2665 (1974).
(L21) Hopkinson, A. C., Calzmadia, I. G., *Theor. Chim. Acta*, 34, 93 (1974).
(L22) Ichikawa, H., Ogata, M., *Chem. Pharm. Bull.*, 22, 1560 (1974).
(L23) Ikuta, S., Yoshihara, K., Shiokawa, T., *Bull. Chem. Soc. Jpn.*, 48, 2134 (1975).
(L24) Jonkman, H. T., Van der Velde, G. A., Nieuwpoort, W. C., *Chem. Phys. Lett.*, 25, 62 (1974).
(L25) Kao, J.-L., Parker, C. E., Bursey, M M., *Org. Mass Spectrom* , 9, 679 (1974).
(L26) Kollman, P., McKelvey, J., Gund, P., *J. Am. Chem Soc.*, 97, 1640 (1975).
(L27) Kner, C., Lorquet, J. C., Bertingin, A., *Org. Mass Spectrom.*, 8, 387 (1974).
(L28) Mahan, B. H., *Acc. Chem. Res.*, 8, 55 (1975).
(L29) Maier, W F., Reetz, M. T., *J. Am. Chem. Soc.*, 97, 3687 (1975).
(L30) McMaster, B. N., in "Mass Spectrometry", Vol. 3, R. A. W. Johnstone, Sr. Reporter, Specialist Periodical Report, The Chemical Society, London, 1975, p 1.
(L31) Meriet, P., Peyerimhoff, S. D., Buenker, R. J., Shih, S., *J. Am. Chem. Soc.*, 96, 959 (1974).
(L32) Ozkan, I., Chu, S. Y., Goodman, L., *J. Chem. Phys.*, 63, 3195 (1975).
(L33) Parker, C. E., Bursey, M. M., Pedersen, L. G., *Org. Mass Spectrom.*, 9, 204 (1974).
(L34) Pople, J. A., *J. Am. Chem Soc.*, 97, 5306 (1975).
(L35) Radom, L., *Aust. J. Chem.*, 27, 231 (1974).
(L36) Reetz, M. T., Maier, W. F., *Theor. Chim. Acta*, 35, 163 (1974).
(L37) Streitwieser, A., Jr., Williams, J. E., Jr., *J. Am. Chem. Soc.* 97, 191 (1975).
(L38) Wilcox, C. F., Jr., Loew, L. M., Jesaitis, R. G., Belin, S., Hsu, J. N. C., *J. Am. Chem. Soc.*, 96, 4081 (1974).
(L39) Williams, J. E., Streitwieser, A., *J. Am. Chem. Soc.*, 97, 2634 (1975).
(L40) Yarkony, D. R., Schaefer, H. F., *J. Chem. Phys.*, 63, 4317 (1975).
(L41) Yoshihara, K., Kobayashi, M., Ikuta, S., Shiokawa, T., *Bull. Chem. Soc. Jpn*, 48, 2433 (1975).

### Negative Ions

(M1) Ahnell, J. E., Koski, W. S., *J. Chem. Phys.*, 62, 4474 (1975).
(M2) Alexander, R. G., Bigley, D. B., Todd, J. F. J., *J. Chem. Soc., Perkin Trans. 2*, 1836 (1974).
(M3) Alexander, R. G., Bigley, D. B., Turner, R. B., Todd, J. F. J., *J. Chem. Soc., Faraday Trans. 1*, 1212 (1974).
(M4) Bowie, J. H., Ho, A. C., *Aust. J. Chem.*, 26, 2009 (1973).
(M5) Bowie, J. H., Ho, A. C., *J. Chem. Soc., Perkin Trans. 2*, 724 (1975).
(M6) Bowie, J. H., Ho, H. C., *Org. Mass Spectrom.*, 9, 1006 (1974).
(M7) Bowie, J. H., Williams, B. D., in "Mass Spectrometry", A. Maccoll, Ed., Int. Rev. Sci. Series Two, Vol. 5, Butterworths, London, and University Park Press, Baltimore (1975).
(M8) Caledonia, G. E., *Chem. Rev.*, 75, 333 (1975).
(M9) Celotta, R J., Bennett, R. A., Hall, J. L., *J. Chem Phys.*, 60, 1740 (1974).
(M10) Christophorou, L. G., Goans, R. E., *J. Chem Phys.*, 60, 4244 (1974).
(M11) Christophorou, L. G., McCorkle, D. L., Pittman, D., *J. Chem Phys* , 60, 1183 (1974)
(M12) Compton, R N , Reinhardt, P W , Cooper, C. D., *J. Chem Phys.*, 60, 2953 (1974).
(M13) Cooper, C. D., Compton, R N., *J Chem Phys.*, 60, 2424 (1974).
(M14) Cooper, C D., Naff, W T , Compton, R N., *J. Chem. Phys.*, 63, 2752 (1975).
(M15) Cottin, M., Martens, C., *Int J. Mass Spectrom. Ion Phys.*, 16, 369 (1975).

(M16) Franklin, J. L., Harland, P. W., *Ann. Rev. Phys Chem* 25, 485 (1974)
(M17) Fraser, I. W., Garnett, J. L., Gregor, I. K., Jessop, K J., *Org. Mass Spectrom.*, 10, 69 (1975).
(M18) Harland, P. W., Franklin, J. L., *J. Chem. Phys* , 61, 1621 (1974).
(M19) Harland, P. W., Rankin, D W H., Thynne, J C. J , *Int. J. Mass Spectrom. Ion Phys.*, 13, 395 (1974)
(M20) Herbst, E., Patterson, T. A., Lineberger, W. C., *J. Chem. Phys.*, 61, 1300 (1974).
(M21) Hotop, H., Patterson, T. A., Lineberger, W. C., *J. Chem Phys.*, 60, 1806 (1974).
(M22) Lyons, L. E., Palmer, L. D , *Int J. Mass Spectrom Ion Phys.*, 16, 431 (1975).
(M23) McCulloh, K. E., Walker, J. A., *Chem. Phys. Lett.*, 25, 439 (1974).
(M24) Moseley, J. T., Bennett, R. A., Peterson, L. R., *Chem. Phys. Lett.*, 26, 288 (1974).
(M25) Nalley, S. J., Compton, R. N., Schweinler, H. C., Anderson, V. E., *J. Chem. Phys.*, 59, 4125 (1973).
(M26) Nenner, I., Schulz, G. J., *J. Chem. Phys.*, 62, 1747 (1975).
(M27) Refaey, K. M. A., Franklin, J. L., *J. Chem. Phys.*, 61, 733 (1974).
(M28) Rothe, E. W., Tang, S. Y., Reck, G. P., *J. Chem. Phys.*, 62, 3829 (1975).
(M29) Spence, D., Schulz, G. J., *J. Chem. Phys.*, 60, 216 (1974).
(M30) Stockdale, J. A., Davis, F. J., Compton, R. N., Klots, C. E., *J. Chem. Phys.*, 60, 4279 (1974).
(M31) Tang, S. Y., Rothe, E. W., Reck, G. P., *Int. J. Mass Spectrom Ion Phys.*, 16, 79 (1974).
(M32) Torgerson, D. F., Westmore, J. B., *Can. J. Chem.*, 53, 933 (1975).
(M33) Tsuda, S., Yokohata, A., Umaba, T., *Bull. Chem. Soc. Jpn*, 46, 2273 (1973).
(M34) Van Brunt, R. J., *J. Chem. Phys.*, 60, 3064 (1974).
(M35) Van Brunt, R. J., Kieffer, L. J., *J. Chem. Phys.*, 60, 3057 (1974).
(M36) Wang, J. Ling-Fai, Margrave, J. L., Franklin, J. L., *J. Chem. Phys.*, 61, 1357 (1974).
(M37) Wilson, J. C., Bowie, J. H., *Org. Mass Spectrom.*, 10, 836 (1975).
(M38) Wilson, J. F., Davis, F. J., Nelson, D. R., Compton, R. N., Crawford, O. H., *J. Chem. Phys.*, 62, 4204 (1975).
(M39) Ziesel, J. P., Schulz, G. J., Milhaud, J., *J. Chem. Phys.*, 62, 1936 (1975).

**Field Ionization and Field Desorption**

(N1) Aberth, W., Spindt, C. A., Rogers, K. T., "Record of 11th Symposium on Electron, Ion and Laser Beam Technology", R. F. M. Thornton, Ed., San Francisco Press, Inc., 1971.
(N2) Ajean, B., Beckey, H. D., Maas, A., Nitschke, U., *Appl. Phys.*, 6, 111 (1975).
(N3) Aleksankin, M. M., Lobanov, V. V., *Int. J. Mass Spectrom. Ion Phys.*, 15, 1 (1974).
(N4) Anbar, M., Aberth, W. H., *Anal. Chem.*, 46, 59A (1974).
(N5) Anbar, M., St. John, G. A., *J. Am. Chem. Soc.*, 97, 7195 (1975).
(N6) Anbar, M., St. John, G. A., *Science*, 190, 781 (1975).
(N7) Ardrey, R E., Hibbitt, B., Robertson, A. J. B., Derrick, P. J., Morgan, R. P., Hill, J. T., Baldwin, M. A., *Int. J. Mass Spectrom. Ion Phys.*, 19, in press (1976).
(N8) Barofsky, D. F., Barofsky, E., *Int. J. Mass Spectrom. Ion Phys.*, 14, 3 (1974).
(N9) Beckey, H. D., "Field Ionization and Field Desorption Mass Spectrometry", to be published by Pergamon Press.
(N10) Beckey, H. D., Gierlich, H. H., Heinen, H. J., Hilt, E., *J. Phys. E.*, 8, 355 (1975).
(N11) Beckey, H. D., Schulten, H. R., *Angew. Chem., Int Ed. Engl.*, 14, 403 (1975).
(N12) Beckey, H D., Schulten, H. R., *Fresenius' Z. Anal. Chem.*, 273, 345 (1975).
(N13) Davis, P. R., Bechtold, E., Block, J. H., *Surf. Sci.*, 45, 585 (1974).
(N14) Derrick, P. J., *Org. Mass Spectrom.*, in press (1976).
(N15) Fales, H. M., Milne, G. W A., Winkler, H. U , Beckey, H. D., Damico, J. N., Barron, R., *Anal. Chem.*, 47, 207 (1975).
(N16) Games, D. E., Games, M P., Jackson, A. H., Olavesen, A. H , Rossiter, M., Winterburn, P. J., *Tetrahedran Lett* , 2377 (1974).
(N17) Gierlich, H. H , Heinen, H. J., Beckey, H. D., *Biomed Mass Spectrom.*, 2, 31 (1975).
(N18) Goldenfeld, I V., Korostyshevsky, I. Z., Mischenchuk, B. G., *Int. J. Mass Spectrom. Ion Phys.*, 13, 297 (1974).
(N19) Hanson, G. R., *J. Chem. Phys.*, 62, 1161 (1975)
(N20) Hass, J. R., Sammons, M. C., Bursey, M. M., Kukuch, B. J., Buck, R P , *Org Mass Spectrom.*, 9, 952 (1974).
(N21) Heinen, H J , Gierlich, H H., Beckey, H. D., *J. Phys. E*, 8, 877 (1975).
(N22) Heinen, H. J., Hotzel, Ch., Beckey, H. D., *Int. J Mass Spectrom Ion Phys.*, 13, 55 (1974)
(N23) Heinen, H J., Rollgen, F W., Beckey, H. D., *Z. Naturforsch. A*, 29, 773 (1974)
(N24) Korol, E. N., Lobanov, V. V., Pokrovsky, V A., *Int. J. Mass Spectrom Ion Phys.*, 18, 229 (1975).
(N25) Kummler, D., Schulten, H. R., *Org. Mass Spectrom.*, 10, 813 (1975).
(N26) Large, R., Knof, H., *J. Chem. Soc., Chem. Commun.*, 935 (1974).
(N27) Larsen, L. A., Ritter, D. M., *Inorg. Chem.*, 13, 2284 (1974).
(N28) Lehmann, W. D., Schulten, H R , Beckey, H. D., *Org. Mass Spectrom.*, 7, 1103 (1973).
(N29) Lobanov, V. V., Aleksankin, M. M., Krugłyak, Yu. A., *Int. J. Mass Spectrom. Ion Phys.*, 18, 275 (1975).
(N30) McEwen, C N., Bolinski, A. G., *Biomed. Mass Spectrom.*, 2, 112 (1975).
(N31) Moor, J., Waight, E. S., *Org. Mass Spectrom.*, 9, 903 (1974).
(N32) Olson, K. L., Cook, J. C., Jr., Rinehart, K. L., Jr., *Biomed Mass Spectrom.*, 1, 358 (1974).
(N33) Robertson, A. J. B., *J. Phys. E*, 7, 321 (1974).
(N34) Robertson, A. J. B., Williams, P., *Adv. Mass Spectrom.*, 4, 847 (1968).
(N35) Rollgen, F. W., Beckey, H. D., *Z. Naturforsch A*, 29, 230 (1974).
(N36) Rollgen, F. W., Heinen, H. J., *Int. J. Mass Spectrom. Ion Phys.*, 17, 92 (1975)
(N37) Röllgen, F. W., Heinen, H. J., *Z. Naturforsch. A*, 30, 918 (1975).
(N38) Röllgen, F. W., Levsen, K., Beckey, H. D., *Org Mass Spectrom.*, 10, 737 (1975).
(N39) Röllgen, F. W., Schulten, H. R., *Org. Mass Spectrom.*, 10, 660 (1975).
(N40) Ryska, M., Kuras, M., Mostecky, J., *Int. J. Mass Spectrom. Ion Phys.*, 16, 257 (1975).
(N41) Sammons, M. C., Bursey, M. M., White, C. K., *Anal. Chem.*, 47, 1165 (1975).
(N42) Schulten, H. R., *Biomed. Mass Spectrom.*, 1, 223 (1974).
(N43) Schulten, H. R., in "New Approaches to the Identification of Microorganisms", C. G. Heden, T. Illeni, Ed., John Wiley & Sons, New York, 1974, p 117.
(N44) Schulten, H. R., Beckey, H. D., *Adv. Mass Spectrom.*, 6, 499 (1974).
(N45) Schulten, H. R., Beckey, H. D., *Org. Mass Spectrom.*, 9, 1154 (1974).
(N46) Schulten, H. R., Games, D. E., *Biomed. Mass Spectrom.*, 1, 120 (1974).
(N47) Schulten, H. R., Röllgen, F. W., *Angew. Chem., Int Ed. Engl.*, 14, 561 (1975).
(N48) Schulten, H R., Röllgen, F. W., *Org. Mass Spectrom.*, 10, 649 (1975).
(N49) Schulten, H. R., Schurath, U., *J. Phys. Chem.*, 79, 51 (1975).
(N50) Scolnick, M E., Aberth, W. H., Anbar, M., *Int. J. Mass Spectrom. Ion Phys.*, 17, 139 (1975).
(N51) Solymosi, F., Block, J. H., *Ber. Bunsenges. Phys. Chem.*, 79, 686 (1975).
(N52) Wightman, R. M., Hinton, D. M., Sammons, M. C., Bursey, M. M., *Int. J. Mass Spectrom. Ion Phys.*, 17, 208 (1975).
(N53) Williams, P., Ph.D. Thesis, University of London, 1966.
(N54) Wood, G. W., Lau, P.-Y., Mak, N., *Biomed. Mass Spectrom.*, 1, 425 (1974).
(N55) Wood, G. W., McIntosh, J. M., Lau, P.-Y., *J. Org. Chem.*, 40, 636 (1975).

**Collision Induced Decomposition**

(O1) Appell, J., Horsley, J. A., *J. Chem. Phys.*, 60, 3445 (1974).
(O2) Ast, T., Terwilliger, D. T., Beynon, J. H., Cooks, R G., *J. Chem. Phys.*, 62, 3855 (1975).
(O3) Baer, T., Squires, L., Werner, A. S., *Chem. Phys.*, 8, 325 (1974).
(O4) Beynon, J. H , Cooks, R. G., Keough, T., *Int. J. Mass Spectrom Ion Phys.*, 14, 437 (1974).
(O5) Blumenthal, T , Bowie, J. H , Hart, S. G., *Aust. J. Chem.*, 26, 2019 (1973)
(O6) Borschers, F., Levsen, K., *Org. Mass Spectrom.*, 10, 584 (1975).
(O7) Bowie, J. H., *Aust. J. Chem.*, 26, 2719 (1973)
(O8) Bowie, J. H., *Org. Mass Spectrom.*, 9, 304 (1974)
(O9) Bowie, J. H., Blumenthal, T., *J. Am. Chem Soc.*, 97, 2959 (1975)
(O10) Bowie, J. H , Hart, S. G., *Int J. Mass Spectrom Ion Phys.*, 13, 319 (1974).
(O11) Bowie, J. H., Williams, B. D., *Aust. J Chem.*, 28, 563 (1975).
(O12) Bregman-Reisler, H , Doering, J P., *J. Chem Phys* , 62, 3109 (1975)
(O13) Constantin, E., *Int. J. Mass Spectrom Ion Phys.*, 13, 343 (1974).
(O14) Cooks, R G., Ast, T., Beynon, J. H., *Int. J. Mass Spectrom Ion Phys.*, 16, 348 (1975)
(O15) Cooks, R. G., Beynon, J. H , Litton, J. F., *Org Mass Spectrom.*, 10, 503 (1975)
(O16) Cooks, R. G., Hendricks, L., Beynon, J. H., *Org. Mass Spectrom.*, 10, 625 (1975).
(O17) Cooks, R. G., Terwilliger, D T., Ast, T., Beynon, J. H., Keough, T., *J. Am. Chem. Soc.*, 97, 1583 (1975).
(O18) Dastidar (Mullick), K. R., Barua, A. K , *J. Chem. Phys* , 62, 4373 (1975).
(O19) Giardini-Guidoni, A., Piatania, R., Zocchi, F., *Int. J. Mass Spectrom Ion Phys.*, 13, 453 (1974)
(O20) Keough, T., Beynon, J. H., Cooks, R G., *Int. J. Mass Spectrom. Ion Phys* , 16, 417 (1975).
(O21) Kim, K. C., Uckotter, M., Beynon, J. H., Cooks, R. G., *Int. J. Mass Spectrom Ion Phys.*, 15, 23 (1974).
(O22) Levsen, K., *Org Mass Spectrom.*, 10, 43 (1975)
(O23) Levsen, K., *Org. Mass Spectrom.*, 10, 55 (1975).
(O24) Levsen, K., Beckey, H. D., *Org. Mass Spectrom.*, 9, 570 (1974).
(O25) Levsen, K., McLafferty, F. W., *J. Am. Chem Soc.*, 98, 139 (1974).
(O26) Levsen, K., McLafferty, F. W., *Org. Mass Spectrom.*, 8, 353 (1974).
(O27) Levsen, K., Schwarz, H., *Org. Mass Spectrom.*, 10, 752 (1975)
(O28) Levsen, K., Wipf, H. K., McLafferty, F. W., *Org. Mass Spectrom.*, 8, 117 (1974).
(O29) McLafferty, F. W., Winkler, J., *J. Am. Chem. Soc.*, 96, 5182 (1974).
(O30) Nibbering, N. M M., Nishishita, T., Van de Sande, C. C., McLafferty, F W., *J. Am. Chem. Soc.*, 96, 5668 (1974).
(O31) Nibbering, N. M. M., Van de Sande, C. C., Nishishita, T., McLafferty, F. W., *Org. Mass Spectrom.*, 9, 1059 (1974).
(O32) Sakurai, H., Tatematsu, A , Nakata, H., *Bull. Chem. Soc. Jpn*, 47, 2731 (1974).
(O33) Van de Sande, C. C., McLafferty, F. W., *J. Am. Chem. Soc.*, 97, 2298 (1975).
(O34) Van de Sande, C. C., McLafferty, F. W., *J. Am. Chem. Soc.*, 97, 4613 (1975).
(O35) Van de Sande, C. C., McLafferty, F. W., *J. Am. Chem. Soc.*, 97, 4617 (1975).

**Chemical Ionization**

(P1) Agosta, W. C., Bowen, D. V., Carmier, R. A., Field, F H., *J. Org. Chem.*, 39, 1752 (1974).
(P2) Bowen, D. V., Field, F. H., *Anal. Chem.*, 47, 2289 (1975).
(P3) Bowen, D. V., Field, F. H., *Org. Mass Spectrom.*, 9, 195 (1974).
(P4) Buttrill, Jr., S. E., Findels, A. F., *Anal. Chem.*, in press (1976).
(P5) Carroll, D. I., Dzidic, I., Stillwell, R. N., Horning, E. C., *Anal. Chem.*, 47, 1956 (1975).
(P6) Carroll, D. I., Dzidic, I., Stillwell, R. N., Horning, M. G., Horning, E. C., *Anal. Chem.*, 46, 706 (1974).
(P7) Chao, J. M., Saferstein, R., Manura, J., *Anal. Chem.*, 46, 296 (1974).
(P8) Dougherty, R. C., Roberts, J. D., Binkley, W. W., Chizhov, O S., Kadentsev, V. I., Solovyov, A. A., *J. Org. Chem* , 39, 451 (1974).
(P9) Dzidic, I., Carroll, D. I., Stillwell, R. N., Horning, E. C., *Anal Chem.*, 47, 1308 (1975).
(P10) Dzidic, I., Carroll, D. I., Stillwell, R. N., Horning, E. C., *J. Am Chem Soc.*, 96, 5258 (1974).
(P11) Gillis, R. G., Lacey, M J., Shannon, J. S., *Org Mass Spectrom.*, 9, 359 (1974).
(P12) Gray, A L., *Analyst (London)*, 100, 289 (1975).
(P13) Gray, A L., *Anal Chem* , 47, 600 (1975)
(P14) Haegele, K. D., Desideno, D. M., Jr., *J. Org. Chem* , 39, 1078 (1973).
(P15) Harrison, A. G., Lin, P.-H., *Can. J. Chem.*, 53, 1314 (1975)
(P16) Hendricks, L. J., Shapiro, R H., *Int J. Mass Spectrom. Ion Phys.*, 15, 399 (1974)

(P17) Horning, E. C., Carroll, D. I., Dzidic, I., Haegele, K. D., Horning, M. G., Stillwell, R. N., *J. Chromatogr. Sci.*, 12, 725 (1974)
(P18) Horning, E. C., Carroll, D. I., Dzidic, I., Haegele, K. D., Horning, M. G., Stillwell, R. N., *J. Chromatogr.*, 99, 13 (1974).
(P19) Horning, E. C., Horning, M. G., Carroll D. I., Dzidic, I., Stillwell, R. N., *Anal. Chem.*, 45, 936 (1973).
(P20) Hunt, D. F., Harvey, T. M., *Anal Chem.*, 47, 1965 (1975).
(P21) Hunt, D. F., Harvey, T. M., *Anal. Chem.*, 47, 2136 (1975).
(P22) Hunt, D. F., Harvey, T. M., Russell, J. W., *J. Chem Soc., Chem. Commun*, 151 (1975).
(P23) Hunt, D. F., McEwen, C. N., Harvey, T. M., *Anal Chem.*, 47, 1730 (1975).
(P24) Jardine, I., Fenselau, C., *Anal. Chem.*, 47, 730 (1975).
(P25) Jardine, I., Fenselau, C., *Org. Mass Spectrom.*, 10, 748 (1975).
(P26) Jelus, B. L., Michnowicz, J., Munson, B., *J. Org. Chem.*, 39, 2130 (1974).
(P27) Jelus, B., Munson, B., Fenselau, C., *Anal. Chem.*, 46, 729 (1974).
(P28) Jelus, B. L., Munson, B., Fenselau, C., *Biomed. Mass Spectrom*, 1, 96, (1974).
(P29) Jelus, B. L., Murray, R. K., Munson, B., *J. Am Chem. Soc.*, 97, 2362 (1975).
(P30) Karasek, F. W., *Anal. Chem.*, 46, 710A (1974).
(P31) Karasek, F. W., Denney, D. W., *Anal. Chem.*, 46, 1312 (1974).
(P32) Karasek, F. W., Denney, D. W., *Anal. Chem.*, 46, 633 (1974).
(P33) Karasek, F. W., Denney, D. W., DeDecker, E. H., *Anal. Chem.*, 46, 970 (1974).
(P34) Levonowich, P. F., Tannenbaum, H. D., Dougherty, R. C., *J. Chem. Soc., Chem. Commun.*, 597 (1975).
(P35) Lias, S. G., Visconi, A., Field, F. H., *J. Am. Chem. Soc.*, 98, 359 (1974).
(P36) Liehr, J. G., McCloskey, J. A., *Org. Mass Spectrom.*, 9, 491 (1974).
(P37) McKeown, M., Siegel, M. W., *Am. Lab.*, 7(11), 89 (1975).
(P38) Meisels, G. G., Sroka, G. J., Mitchum, R. K., *J. Am. Chem. Soc.*, 96, 5045 (1974).
(P39) Michnowicz, J., Munson, B., *Org. Mass Spectrom.*, 8, 49 (1974).
(P40) Milne, G. W. A., Lacey, M. J., *Crit. Rev. Anal. Chem.*, 4, 45 (1974).
(P41) Mitchum, R. K., Freeman, J. P., Meisels, G. G., *J. Chem. Phys.*, 62, 2485 (1975).
(P42) Pierce, R. C., Porter, R. F., *J. Phys. Chem.*, 78, 93 (1974).
(P43) Price, P., Martinsen, D. P., Upham, R. A., Swofford, H. S. Jr., Buttrill, S. G. Jr., *Anal. Chem.*, 47, 190 (1975).
(P44) Risby, T. H., Jura, P. C., Lampe, F. W., Yergey, A. L., *Anal. Chem.*, 46, 161 (1974).
(P45) Risby, T. H., Jura, P. C., Lampe, F. W., Yergey, A. L., *Anal. Chem.*, 46, 726 (1974).
(P46) Tannenbaum, H. D., Roberts, J. D., Dougherty, R. C., *Anal. Chem.*, 47, 49 (1975).
(P47) Tumlinson, J. H., Heath, R. R., Doolittle, R. C., *Anal. Chem.*, 46, 1309 (1974).
(P48) Volkov, N. F., Karachevtsev, G. V., Marutkin, A. Z., Kholodov, A. I., *Instrum. Exp. Tech.*, 17, 631 (1974).
(P49) Weinkam, R. J., *J. Am. Chem. Soc.*, 96, 1032 (1974).
(P50) Wilson, J. M., in "Mass Spectrometry", Vol. 3, A Specialist Periodical Report, R. A. W. Johnstone, Sr. Reporter, The Chemical Society, London, 1975, p 86.
(P51) Wilson, M. S., McCloskey, J. A., *J. Am. Chem. Soc.*, 97, 3436 (1975).
(P52) Yu, T. Y., Field, F. H., *Org. Mass Spectrom.*, 8, 267 (1974).

### High Pressure Mass Spectrometry

(Q1) Chin Lin, M. S., Harrison, A. G., *Int. J. Mass Spectrom. Ion Phys.*, 17, 97 (1975).
(Q2) Dougherty, R. C., Dalton, J., Roberts, J. D., *Org. Mass Spectrom.*, 8, 77 (1974).
(Q3) Dougherty, R. C., Roberts, J. D., *Org. Mass Spectrom.*, 8, 81 (1974).
(Q4) Dougherty, R. C., *Org. Mass Spectrom.*, 8, 85 (1974).
(Q5) Heckel, E., Hanrahan, R. J., *J. Chem. Phys.*, 62, 1027 (1975).
(Q6) Hiraoka, K., Kebarle, P., *Can. J. Chem.*, 53, 970 (1975).
(Q7) Hiraoka, K., Kebarle, P., *J. Am. Chem. Soc.*, 97, 4179 (1975).
(Q8) Hiraoka, K., Kebarle, P., *J. Chem. Phys.*, 62, 2267 (1975)
(Q9) Hiraoka, K., Kebarle, P., *J. Chem. Phys.*, 63, 394 (1975).
(Q10) Hiraoka, K., Kebarle, P., *J. Chem. Phys.*, 63, 746 (1975).
(Q11) Jones, E. G., Bhattacharya, A. K., Tiernan, T. O., *Int. J. Mass Spectrom. Ion Phys.*, 17, 147 (1975).
(Q12) Klevan, L., Munson, B., *Int. J. Mass Spectrom. Ion Phys.*, 13, 261 (1974).
(Q13) Luczynski, Z., Malicki, W., Wincel, H., *Int. J. Mass Spectrom. Ion Phys.*, 15, 321 (1974).
(Q14) Luczynski, Z., Wincel, H., *Int. J. Mass Spectrom. Ion Phys.*, 14, 29 (1974).
(Q15) Mackenzie Peers, A., *Int. J. Mass Spectrom Ion Phys.*, 14, 155 (1974).
(Q16) McMahon, T. B., Kebarle, P., *J. Am. Chem. Soc.*, 96, 5940 (1974).
(Q17) Meot-Ner, M., Field, F. H., *J. Am. Chem. Soc.*, 97, 2014 (1975).
(Q18) Meot-Ner, M., Field, F. H., *J. Am. Chem. Soc.*, 97, 5339 (1975).
(Q19) Meot-Ner, M., Field, F. H., *J. Chem. Phys.*, 61, 3742 (1974).
(Q20) Meot-Ner, M., Solomon, J. J., Field, F. H., Gershinowitz, H., *J. Phys. Chem.*, 78, 1773 (1974).
(Q21) Mlasek, P. G., Beauchamp, J. L., *Int. J. Mass Spectrom. Ion Phys.*, 15, 49 (1974).
(Q22) Mlasek, P. G., Harrison, A. G., *J. Am. Chem. Soc.*, 97, 714 (1975).
(Q23) Reuben, B. G., *Int. J. Mass Spectrom. Ion Phys.*, 13, 181 (1974).
(Q24) Ryan, K. R., *J. Chem. Phys.*, 61, 1559 (1974).
(Q25) Schnitzer, R., Klein, F. S., *Int. J. Mass Spectrom. Ion Phys.*, 16, 377 (1975).
(Q26) Solka, B. H., Harrison, A. G., *Int. J. Mass Spectrom. Ion Phys.*, 14, 125 (1974).
(Q27) Solka, B. H., Harrison, A. G., *Int. J. Mass Spectrom. Ion Phys.*, 14, 295 (1974).
(Q28) Solka, B. H., Harrison, A. G., *Int. J. Mass Spectrom. Ion Phys.*, 17, 379 (1975).
(Q29) Solka, B. H., Lau, A. Y.-K., Harrison, A. G., *Can. J. Chem.*, 52, 1798 (1974).
(Q30) Solomon, J. J., Field, F. H., *J. Am. Chem. Soc.*, 97, 2625 (1975).
(Q31) Su, T., Bowers, M. T., *Int. J. Mass Spectrom. Ion Phys.*, 17, 309 (1975).
(Q32) Tang, I. N., Castleman, A. W., Jr., *J. Chem. Phys.*, 60, 3981 (1974).
(Q33) Yamdagni, R., Kebarle, P., *Ber. Bunsenges. Phys. Chem.*, 78, 181 (1974).
(Q34) Yamdagni, R., Kebarle, P., *Can. J. Chem.*, 52, 861 (1974).
(Q35) Zielinska, T. J., Wincel, H., *Chem. Phys. Letters*, 25, 354 (1974).

### Ion Cyclotron Resonance

(R1) Anicich, V. G., Bowers, M. T., *Int. J. Mass Spectrom. Ion Phys.*, 13, 351 (1974).
(R2) Anicich, V. G., Bowers, M. T., *Int. J. Mass Spectrom. Ion Phys.*, 13, 359 (1974).
(R3) Anicich, V. G., Bowers, M. T., *J. Am. Chem. Soc.*, 96, 1279 (1974).
(R4) Anicich, V. G., Futrell, J. H., Huntress, W. T., Kim, J. K., *Int. J. Mass Spectrom. Ion Phys.*, 18, 63 (1975).
(R5) Aoyagi, K., *Bull. Chem. Soc. Jpn*, 47, 519 (1974).
(R6) Arnett, E. M., Johnston, D. E., Small, L. E., *J. Am. Chem. Soc.*, 97, 5598 (1975).
(R7) Arnett, E. M., Small, L. E., McIver, R. T. Jr., Miller, J. S., *J. Am. Chem. Soc.*, 96, 5638 (1974).
(R8) Arshadi, M. R., Futrell, J. H., *J. Phys. Chem.*, 78, 1482 (1974).
(R9) Asubiojo, O. I., Blair, L. K., Brauman, J. I., *J. Am. Chem. Soc.*, 97, 6685 (1975).
(R10) Aue, D. H., Webb, H. M., Bowers, M. T., *J. Am. Chem. Soc.*, 97, 4136 (1975).
(R11) Beauchamp, J. L., Caserio, M. C., McMahon, T. B., *J. Am. Chem. Soc.*, 96, 6243 (1974).
(R12) Bordwell, F. G., Bartmess, J. E., Drucker, G. E., Margolin, Z., Matthews, W. S., *J. Am. Chem. Soc.*, 97, 3226 (1975).
(R13) Bowers, M. T., Kemper, P. R., Lauderslager, J. B., *J. Chem Phys.*, 61, 4394 (1974).
(R14) Bowie, J. H., *Aust. J. Chem.*, 28, 559 (1975).
(R15) Bowie, J. H., Williams, B. D., *Aust. J. Chem.*, 27, 769 (1974).
(R16) Bowie, J. H., Williams, B. D., *Aust. J. Chem.*, 27, 1923 (1974).
(R17) Bowie, J. H., Williams, B. D., *Int. J. Mass Spectrom Ion Phys.*, 17, 395 (1975).
(R18) Bowie, J. H., Williams, B. D., *Org. Mass Spectrom*, 10, 141 (1975)
(R19) Blunt, R. J., McMahon, T. B., Beauchamp, J. L., *J. Am Chem Soc*, 96, 1269 (1974).
(R20) Briscese, S. M. J., Riveros, J. M., *J. Am Chem. Soc.*, 95, 230 (1975).
(R21) Chatfield, D. A., Bursey, M. M., *Int. J. Mass Spectrom. Ion Phys.*, 18, 239 (1975).
(R22) Chatfield, D. A., Bursey, M. M., *J. Am Chem Soc.*, 97, 3600 (1975).
(R23) Comisarow, M. B., Marshall, A. G., *Can. J Chem.*, 52, 1997 (1974).
(R24) Comisarow, M. B., Marshall, A. G., *Chem Phys Lett.*, 25, 282 (1974).
(R25) Comisarow, M. B., Marshall, A. G., *Chem Phys. Lett.*, 26, 489 (1974).
(R26) Comisarow, M. B., Marshall, A. G., *J. Chem. Phys.*, 62, 293 (1975).
(R27) Dunbar, R. C., *J. Am. Chem. Soc.*, 97, 1382 (1975).
(R28) Dunbar, R. C., Bursey, M. M., Chatfield, D. A., *Int. J. Mass Spectrom. Ion Phys.*, 13, 195 (1974)
(R29) Dymerski, P. P., Fu, E., Dunbar, R. C., *J Am. Chem. Soc.*, 96, 4109 (1974).
(R30) Dymerski, P. P., Dunbar, R. C., Dugan, J. V., Jr., *J. Chem. Phys.*, 61, 298 (1974).
(R31) Foster, M. S., Beauchamp, J. L., *J Am Chem. Soc.*, 97, 4808 (1975).
(R32) Foster, M. S., Beauchamp, J. L., *J. Am Chem. Soc.*, 97, 4814 (1975).
(R33) Freiser, B. S., Beauchamp, J. L., *J Am Chem. Soc.*, 96, 6260 (1974).
(R34) Freiser, B. S., Woodin, R. L., Beauchamp, J. L., *J. Am. Chem. Soc.*, 97, 6893 (1975).
(R35) Grant, B., Djerassi, C., *J. Am. Chem. Soc.*, 96, 3477 (1974).
(R36) Gross, M. L., Lin, P.-H., *Org. Mass Spectrom.*, 9, 1194 (1974).
(R37) Hehre, W. J., McIver, R. T., Jr., Pople, J. A., Schleyer, P. v. R., *J. Am. Chem. Soc.*, 96, 7162 (1974).
(R38) Henion, J. D., Kao, J.-I., Nixon, W. B., Bursey, M. M., *Anal. Chem.*, 47, 689 (1975).
(R39) Huntress, W. T., Jr., Laudenslager, J. B., Pinizzotto, R. F., Jr., *Int. J. Mass Spectrom. Ion Phys.*, 13, 331 (1974).
(R40) Jaffe, S., Klein, F. S., *Int. J. Mass Spectrom. Ion Phys.*, 14, 459 (1974).
(R41) Karpas, Z., Klein, F. S., *Int. J. Mass Spectrom. Ion Phys.*, 16, 289 (1975).
(R42) Karpas, Z., Klein, F. S., *Int. J. Mass Spectrom. Ion Phys.*, 18, 65 (1975).
(R43) Kim, J. K., Theard, L. P., Huntress, W. T., Jr., *J. Chem Phys.*, 62, 45 (1975).
(R44) Kim, J. K., Huntress, W. T., Jr., *J. Chem. Phys.*, 62, 2820 (1975).
(R45) Kim, J. K., Pau, J. K., Caserio, M. C., *J. Chem. Soc., Chem. Commun.*, 121 (1974).
(R46) Kramer, J. M., Dunbar, R. C., *J. Chem. Phys.*, 60, 5122 (1974).
(R47) Laudenslager, J. B., Huntress, W. T., *Int. J. Mass Spectrom. Ion Phys.*, 14, 435 (1974).
(R48) Laudenslager, J. B., Huntress, W. T., Jr., Bowers, M. T., *J. Chem. Phys.*, 61, 4600 (1974).
(R49) LeBreton, P. R., Williamson, A. D., Beauchamp, J. L., Huntress, W. T., *J. Chem. Phys.*, 62, 1623 (1975).
(R50) Lieder, C. A., Brauman, J. I., *Int. J. Mass Spectrom. Ion Phys.*, 16, 307 (1975).
(R51) Marshall, A. G., Comisarow, M. B., *Anal Chem.*, 47, 491A (1975).
(R52) McAllister, T., *Int. J. Mass Spectrom. Ion Phys.*, 13, 63 (1974).
(R53) McAllister, T., *Int. J. Mass Spectrom. Ion Phys.*, 16, 303 (1974).
(R54) McIver, R. T., *Org. Mass Spectrom.*, 10, 396 (1975).
(R55) McIver, R. T., Baranyi, A. D., *Int. J. Mass Spectrom. Ion Phys.*, 14, 449 (1974).
(R56) McIver, R. T., Jr., Ledford, E. B., Jr., Miller, J. S., *Anal. Chem.*, 47, 692 (1975).
(R57) Morton, T. H., Beauchamp, J. L., *J. Am. Chem. Soc.*, 97, 2355 (1975).
(R58) Pasto, D. J., *J. Am. Chem. Soc.*, 97, 136 (1975).
(R59) Peshack, C. V., Buttrill, S. E., *J. Am. Chem Soc.*, 96, 6027 (1974).
(R60) Reed, K. J., Brauman, J. I., *J. Am. Chem Soc.*, 97, 1625 (1975).
(R61) Richardson, J. H., Stephenson, L. M., Brauman, J. I., *Chem. Phys. Lett.*, 25, 318 (1974).
(R62) Richardson, J. H., Stephenson, L. M., Brauman, J. I., *Chem. Phys Lett.*, 25, 321 (1974)
(R63) Richardson, J. H., Stephenson, L. M., Brauman, J. I., *J. Am. Chem Soc.*, 97, 1160 (1975)

(R64) Richardson, J. H., Stephenson, L. M., Brauman, J. I., *J. Am. Chem. Soc.*, 97, 2967 (1975).
(R65) Richardson, J. H., Stephenson, L. M., Brauman, J. I., *J. Chem. Phys.*, 62, 1580 (1975).
(R66) Richardson, J. H., Stephenson, L. M., Brauman, J. I., *J. Chem. Phys.*, 63, 74 (1975).
(R67) Ridge, D. P., *J. Am. Chem. Soc.*, 97, 5670 (1975).
(R68) Ridge, D. P., Beauchamp, J. L., *J. Am. Chem Soc.*, 96, 637 (1974).
(R69) Selcik, M. D., Henis, J. M. S., Gaspar, P. P., *J. Chem Phys.*, 61, 4321 (1974).
(R70) Selcik, M. D., Henis, J. M. S., Gaspar, P. P., *J. Chem. Phys.*, 61, 4329 (1974).
(R71) Shen, J., Dunbar, R. C., Olah, G. A., *J. Am. Chem Soc.*, 96, 6227 (1974).
(R72) Smith, D. L., Futrell, J. H., *J. Phys. B.*, 8, 803 (1975).
(R73) Staley, R. H., Beauchamp, J. L., *J. Am. Chem. Soc.*, 96, 6252 (1974).
(R74) Staley, R. H., Beauchamp, J. L., *J. Chem. Phys*, 62, 1998 (1975).
(R75) Su, T., Bowers, M. T., *J. Chem. Phys.*, 60, 4897 (1974).
(R76) Tiedemann, P. W., Riveros, J. M., *J. Am. Chem. Soc.*, 96, 185 (1974).
(R77) Tomer, K. B., *Org. Mass Spectrom.*, 9, 686 (1974).
(R78) Vogt, J., Beauchamp, J. L., *J. Am. Chem. Soc.*, 97, 6682 (1975).
(R79) Wanczek, K.-P., *Z. Naturforsch. A*, 30, 329 (1975).
(R80) Wanczek, K.-P., Profous, Z.-C., *Int. J. Mass Spectrom. Ion Phys.*, 17, 23 (1975).
(R81) Wieting, R. D., Staley, R. H., Beauchamp, J. L., *J. Am. Chem. Soc.*, 97, 924 (1975).
(R82) Wieting, R. D., Staley, R. H., Beauchamp, J. L., *J. Am. Chem. Soc.*, 96, 7552 (1974).
(R83) Williamson, A. D., Beauchamp, J. L., *J. Am. Chem. Soc.*, 97, 5714 (1975).
(R84) Wilson, J. C., Bowie, J. H., *Aust. J. Chem.*, 28, 1993 (1975).
(R85) Wolf, J. F., Harch, P. G., Taft, R. W., Hehre, W. J., *J. Am. Chem. Soc.*, 97, 2902 (1975).

**Tandem Mass Spectrometers and Beams**

(S1) Ardelean, P., Mercea, V., *Int. J. Mass Spectrom. Ion Phys.*, 18, 201 (1975).
(S2) Cheng, T. M. H., Yu, T.-Y., Lampe, F. W., *J. Phys. Chem.*, 78, 1184 (1974).
(S3) Dimpfl, W. L., Mahan, B. H., *J. Chem. Phys.*, 60, 3238 (1974).
(S4) Flaux, A., Smith, D. L., Futrell, J. H., *Int. J. Mass Spectrom. Ion Phys.*, 15, 9 (1974).
(S5) Henis, J. M. S., Tripodi, M. K., *J. Chem. Phys.*, 61, 4863 (1974).
(S6) Jonsson, B.-O., Lind, J., *J. Chem. Soc., Faraday Trans. 2*, 1399 (1974).
(S7) Lehrle, R. S., Parker, J. E., *Int. J. Mass Spectrom. Ion Phys.*, 15, 133 (1974).
(S8) Mayer, T. M., Lampe, F. W., *J. Phys. Chem.*, 78, 2195 (1974).
(S9) Mayer, T. M., Lampe, F. W., *J. Phys. Chem.*, 78, 2422 (1974).
(S10) Mayer, T. M., Lampe, F. W., *J. Phys. Chem.*, 78, 2429 (1974).
(S11) Mayer, T. M., Lampe, F. W., *J. Phys. Chem.*, 78, 2433 (1974).
(S12) Mayer, T. M., Lampe, F. W., *J. Phys. Chem.*, 78, 2645 (1974).
(S13) Milner, R. G., Parker, J. E., *Int. J. Mass Spectrom. Ion Phys.*, 17, 185 (1975).
(S14) Rayborn, G. H., Bailey, T. L., *J. Chem. Phys.*, 60, 813 (1974).
(S15) Smith, D. L., Futrell, J. H., *Int. J. Mass Spectrom. Ion Phys.*, 14, 171 (1974).
(S16) Smith, G. P. K., Cross, R. J., Jr., *J. Chem. Phys.*, 60, 2125 (1974).
(S17) Smith, G. P. K., Carlson, R. D., Cross, R. J., Jr., *J. Chem. Phys.*, 62, 1999 (1975).
(S18) Smith, G. P. K., Weiner, J., Saunders, M., Cross, R. J., Jr., *J. Am. Chem. Soc.*, 97, 3593 (1975).
(S19) Wyatt, J. R., Strattan, L. W., Snyder, S. C., Hierl, P. M., *J. Chem. Phys.*, 60, 3702 (1974).
(S20) Wyatt, J. R., Strattan, L. W., Snyder, S. C., Hierl, P. M., *J. Chem. Phys.*, 62, 2555 (1975).

**Flowing Afterglow and Drift Tubes**

(T1) Bierbaum, V. M., Kaufman, F., *J. Chem. Phys.*, 61, 3804 (1974).
(T2) Fehsenfeld, F. C., *Int. J. Mass Spectrom. Ion Phys*, 16, 151 (1975).
(T3) Fehsenfeld, F. C., *J. Chem. Phys.*, 61, 1588 (1974).
(T4) Fehsenfeld, F. C., Albritton, D. L., Bush, Y. A., Fournier, P. G., Govers, T. R., Fournier, J., *J. Chem. Phys*, 61, 2150 (1974).
(T5) Fehsenfeld, F. C., Ferguson, E. E., *J. Chem. Phys.*, 61, 3181 (1974).
(T6) Fehsenfeld, F. C., Howard, C. J., Schmeltekopf, A. L., *J. Chem Phys.*, 63, 2835 (1975).
(T7) Fehsenfeld, F. C., Lindinger, W., Albritton, D. L., *J. Chem. Phys.*, 63, 443 (1975).
(T8) Fehsenfeld, F. C., Lindinger, W., Schmeltekopf, A. L., Albritton, D. L., Ferguson, E. E., *J. Chem. Phys.*, 62, 2001 (1975).
(T9) Helmerl, J. M., Vanderhoff, J. A., *J. Chem Phys.*, 60, 4362 (1974).
(T10) Hemsworth, R. S., Payzant, J. D., Schiff, H. I., Bohme, D. K., *Chem. Phys. Lett.*, 26, 417 (1974)
(T11) Horton, R. L., Franklin, J. L., Mazzeo, B., *J. Chem Phys.*, 62, 1739 (1975).
(T12) Johnsen, R., Huang, C. M., Biondi, M. A., *J. Chem. Phys.*, 63, 3374 (1975).
(T13) Lindinger, W., Albritton, D. L., *J. Chem. Phys.*, 62, 3517 (1975).
(T14) Lindinger, W., Albritton, D. L., Fehsenfeld, F. C., Schmeltekopf, A. L., Ferguson, E. E., *J. Chem. Phys.*, 62, 3549 (1975).
(T15) Lindinger, W., Albritton, D. L., McFarland, M., Fehsenfeld, F. C., Schmeltekopf, A. L., Ferguson, E. E., *J. Chem. Phys.*, 62, 4101 (1975).
(T16) Lindinger, W., Albritton, D. L., Howard, C. J., Fehsenfeld, F. C., Ferguson, E. E., *J. Chem. Phys.*, 63, 5220 (1975).
(T17) Lindinger, W., McFarland, M., Fehsenfeld, F. C., Albritton, D. L., Schmeltekopf, A. L., Ferguson, E. E., *J. Chem. Phys.*, 63, 2175 (1975).
(T18) Liu, W. F., Conway, D. C., *J. Chem. Phys.*, 62, 3070 (1975).
(T19) Schiff, H. I., Bohme, D. K., *Int. J. Mass Spectrom. Ion Phys.*, 16, 167 (1975).
(T20) Tang, I. N., Castleman, A. W., *J. Chem. Phys.*, 62, 4576 (1975).

**Amino Acids, Peptides, Protein-Sequencing**

(U1) Asante-Poku, S., Wood, G. W., Schmidt, D. E., Jr., *Biomed. Mass Spectrom.*, 2, 121 (1975).
(U2) Beuhler, R. J., Flanigan, E., Greene, L. J., Friedman, L., *Biochemistry*, 13, 5060 (1974).
(U3) Beuhler, R. J., Flanigan, E., Greene, L. J., Friedman, L., *J. Am. Chem. Soc.*, 96, 3990 (1974).
(U4) Bowen, D. V., Field, F. H., 22nd Annual Conference on Mass Spectrometry and Allied Topics, Philadelphia, Pa., May 1974, p 298.
(U5) Dell, A., Morris, H. R., *Biochem. Biophys. Res. Commun.*, 61, 1125 (1974).
(U6) Dell, A., Morris, H. R., Williams, D. H., Ambler, R. P., *Biomed. Mass Spectrom.*, 1, 296 (1974).
(U7) Falter, H., Jayasimhulu, K., Day, R. A., *Anal. Biochem.*, 67, 359 (1975).
(U8) Felker, P., Bandurski, R. S., *Anal. Biochem.*, 67, 245 (1975).
(U9) Grahl-Nielsen, O., Solheim, E., *Anal. Chem.*, 47, 333 (1975).
(U10) Guyer, R. L., Schnute, W. C., Jr., Todd, C. W., Lovins, R. E., *Anal. Biochem.*, 66, 623 (1975).
(U11) Haegele, K. D., Holzer, G., Parr, W., Nakagawa, S. H., Desiderio, D. M., *Biomed. Mass Spectrom.*, 1, 175 (1974).
(U12) Hass, G. M., Nau, H., Biemann, K., Grahn, D. T., Ericsson, L. H., Neurath, H., *Biochemistry*, 14, 1334 (1975).
(U13) Hirota, H., *Biomed. Mass Spectrom.*, 1, 175 (1974).
(U14) Horman, I., Hesford F. J., *Biomed Mass. Spectrom.*, 1, 115 (1974).
(U15) Johnstone, R. A. W., Povall, T. J., *J. Chem. Soc., Perkin Trans. 1*, 13, 1297 (1975).
(U16) Kelley, J. A., Nau, H., Förster, H.-J., Biemann, K., *Biomed. Mass Spectrom.*, in press, 1976.
(U17) Levsen, K., Wipf, H.-K., McLafferty, F. W., *Org. Mass Spectrom.*, 8, 117 (1974).
(U18) Merritt, C., Jr., DiPietro, C., Robertson, D. H., Levy, E. J., *J. Chromatogr. Sci.*, 12, 668 (1974)
(U19) Morris, . H. R., *Biochem. Soc. Trans.*, 2, 806 (1974).
(U20) Morris, H. R., Williams, D. H., Midwinter, G. G., Hartley, B. S., *Biochem. J.*, 141, 701 (1974).
(U21) Mudgett, M., Bowen, D. V., Kindt, T. J., Field, F. H., *Biomed. Mass Spectrom*, 2, 254 (1975).
(U22) Mural, A., Takeuchi, Y., *Bull. Chem. Soc. Jpn*, 48, 2911 (1975).
(U23) Nau, H., *Biochem. Biophys. Res. Commun.*, 59, 1088 (1974).
(U24) Nau, H., Forster, H.-J., Kelley, J. A., Biemann, K., *Biomed. Mass Spectrom.*, in press, 1976.
(U25) Nau, H., Riordan, F., *Biochemistry*, 14, 5285 (1975).
(U26) Okada, K., Nagai, S., Uyehara, T., Hiramoto, M., *Tetrahedron*, 30, 1175 (1974).
(U27) Pritchard, D. G., Schnute, W. C., Jr., Todd, C. W., *Biochem. Biophys. Res. Commun.*, 65, 312 (1975).
(U28) Rangarajan, M., Ardrey, R. E., Darbre, A., *J. Chromatogr.*, 87, 499 (1973).
(U29) Rapp, U., Maurer, K. H., Schafer, W., 22nd Annual Conference on Mass Spectrometry and Allied Topics, Philadelphia, Pa., May 1974, 301.
(U30) Roepstorff, P., Kristiansen, K., *Biomed. Mass Spectrom.*, 1, 231 (1974).
(U31) Schier, G. M., Halpern, B., *Aust. J. Chem.*, 27, 393 (1974).
(U32) Schier, G. M., Halpern, B., *Aust. J. Chem.*, 27, 2455 (1974).
(U33) Schier, G. M., Halpern, B., Milne, G. W., *Biomed. Mass Spectrom.*, 1, 212 (1974).
(U34) Schulman, M. F., Abramson, F. P., *Biomed. Mass Spectrom.*, 2, 9 (1975).
(U35) Summons, R. E., Pereira, W. E., Reynolds, W. E., Rindfleisch, T. C., Duffield, A. M., *Anal. Chem.*, 46, 582 (1974).
(U36) van't Klooster, H. A., Vaarkamp-Lijnse, J. S., Dijkstra, G., *Adv. Mass Spectrom.*, 6, 1027 (1974).

**Purines and Pyrimidines, Nucleosides, Nucleotides**

(V1) Bryant, W. F., Klein, P. D., *Anal. Biochem.*, 65, 73 (1975).
(V2) Chheda, G. B., Dutta, S. P., Mittelman, A., Baczynskj, L., *Tetrahedron Lett.*, 5, 433 (1974).
(V3) Hattox, S. E., McCloskey, J. A., *Anal. Chem.*, 46, 1378 (1974).
(V4) Kempster, E. J., Heck, H. d'A., McReynolds, J. H., Anbar, M., 22nd Annual Conference on Mass Spectrometry and Allied Topics, May 1974, Philadelphia, Pa., 310.
(V5) Liehr, J. G., von Minden, D. L., Hattox, S. E., McCloskey, J. A., *Biomed Mass Spectrom.*, 1, 281 (1974).
(V6) Ludlam, D. B., Kramer, B. S., Wang, J., Fenselau, C., *Biochemistry*, 14, 5480 (1975).
(V7) McCloskey, J. A., in "Basic Principles in Nucleic Acid Chemistry", Vol. 1, P. O. P. Ts'o, Ed., Academic Press, New York, 1974, p 209.
(V8) McCloskey, J. A., Barnes, L. B., Crain, P. F., Lyman, K. J., Bishop, S. H., *Biomed. Mass Spectrom.*, 2, 90 (1975).
(V9) Pantarotto, C., Martini, A., Belvedere, G., Bossi, A., Donelli, M. G., Frigerio, A., *J. Chromatogr.*, 99, 519 (1974).
(V10) Posthumus, M. A., Nibbering, N. M., Boerboom, A. J., Schulten, H.-R., *Biomed. Mass Spectrom.*, 1, 352 (1974).
(V11) Quilliam, M. A., Ogilvie, K. K., Westmore, J. B., *Biomed. Mass Spectrom.*, 1, 78 (1974).
(V12) Ro-Choi, T. S., Choi, Y. C., Henning, D., McCloskey, J., Busch, H., *J. Biol. Chem.*, 250, 3921 (1975).
(V13) von Minden, D. L., Liehr, J. G., Wilson, M. H., McCloskey, J. A., *J. Org. Chem.*, 39, 285 (1974).
(V14) Wilson, M. S., McCloskey, J. A., *J. Am. Chem. Soc.*, 97, 3436 (1975).

**Carbohydrates**

(W1) Aspinall, G. O., Tam, S. C., *Carbohydr. Res.*, 38, 71 (1974).
(W2) Björndal, H., Lindberg, B., Lönngren, J., Mészáros, M., Thompson, J. L., Nimmich, W., *Carbohydr. Res.*, 31, 93 (1973)
(W3) Bursey, M. M., Sammons, M. C., *Carbohydr. Res.*, 37, 355 (1974).
(W4) Colard, M. H. M., Dumont, P. A., Compernolle, F., *Biomed. Mass Spectrom.*, 2, 156 (1975).
(W5) Dizdaroglu, M., Henneberg, D., von Sonntag, C., *Org. Mass Spectrom.*, 8, 335 (1974).
(W6) Egge, H., Nicolai, H., Zilliken, F., *FEBS Lett.*, 39, 341 (1974).
(W7) Guerrera, J., Weill, C. E., *Carbohydr. Res.*, 27, 471 (1973).
(W8) Holder, N. L., Fraser-Reid, B., *Tetrahedron*, 29, 4077 (1973).
(W9) Horton, D., Jewell, J. S., Just, E. K., Wander, J. D., Foltz, R. L., *Biomed. Mass Spectrom.*, 1, 145 (1974).
(W10) Horton, D., Wander, J. D., Foltz, R. L., *Carbohydr. Res.*, 36, 75 (1974).
(W11) Kováčik, V., Kováč, P., *Org Mass Spectrom*, 9, 172 (1974).
(W12) Kováčik, V., Kováč, P., *Carbohydr. Res.*, 38, 25 (1974).

(W13) Kovačik, V., Linek, K., Sandtnerová, R., *Carbohydr. Res.*, 38, 300 (1974).
(W14) Lonngren, J., Svensson, S., *Adv. Carbohydr. Chem Biochem*, 29, 42 (1974)
(W15) Matsubara, T., Hayashi, A., *Biomed. Mass Spectrom*, 1, 62 (1974).
(W16) McGregor, M. L., Reid, R., Waller, G. R., Nelson, E. C., *Spectrosc. Lett*, 7, 45 (1974).
(W17) McKinley, I. R., Weigel, H., *Carbohydr. Res.*, 32, 187 (1974).
(W18) Moor, J., Waight, E. S., *Biomed. Mass Spectrom*, 2, 36 (1975).
(W19) Morgenlie, S., *Carbohydr. Res.*, 41, 285 (1975).
(W20) Orme, T. W., Boone, C. W., Roller, P. P., *Carbohydr. Res.*, 37, 261 (1974).
(W21) Petersson, G., *Carbohydr. Res.*, 43, 1 (1975).
(W22) Reinhold, V. N., Wirtz-Peitz, F., Biemann, K., *Carbohydr. Res.*, 37, 203 (1974).
(W23) Schwarzmann, G. O. H., Jeanloz, R. W., *Carbohydr. Res.*, 34, 161 (1974).
(W24) Sjostrom, E., Pfister, K., Seppala, E., *Carbohydr. Res.*, 38, 293 (1974).
(W25) Szafranek, J., Pfaffenberger, C. D., Horning, E. C., *Carbohydr. Res.*, 38, 97 (1974).
(W26) Tai, T., Yamashita, K., Kobata, A., *J. Biochem.*, 78, 679 (1975).
(W27) Vigevani, A., Gioia, B., Cassinelli, G., *Carbohydr. Res.*, 32, 321 (1974).
(W28) Wood, P. J., Siddiqui, I. R., *Carbohydr. Res.*, 32, 97 (1974).
(W29) Wood, P. J., Siddiqui, I. R., *Carbohydr Res.*, 38, 247 (1974).

**Complex Lipids**

(X1) Batrakov, S. G., Il'ina, E. F., Rozynov, B. V., Bergel'son, L. D., *Bull. Acad. Sci. USSR, Div. Chem. Sci.*, 24, 85 (1975) translated from *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1, 94 (1975).
(X2) Batrakov, S. G., Il'ina, E. F., Rozynov, B. V., Bergel'son, L. D., *Bull. Acad. Sci. USSR, Div. Chem. Sci.*, 23, 2147 (1974); translated from *Izv. Akad. Nauk SSSR, Ser. Khim.*, 10, 2229 (1974).
(X3) Batrakov, S. G., Panosyan, A. G., Konova, I. V., Bergelson, L. D., *Biochim. Biophys. Acta*, 337, 29 (1974).
(X4) Boren, H. B., Garegg, P. J., Kenne, L., Pilotti, A., Svensson, S., Swahn, C.-G., *Acta Chem. Scand.*, 27, 3557 (1973).
(X5) Breimer, M. E., Karlsson, K.-A., Samuelsson, B. E., *Biochim. Biophys. Acta*, 348, 232 (1974).
(X6) Clayton, R. B., Cooper, J. M., Curstedt, T., Sjövall, J., Borsook, H., Chin, J., Schwarz, A., *J. Lipid Res.*, 15, 557 (1974).
(X7) Curstedt, T., Sjövall, J., *Biochim. Biophys. Acta*, 360, 24 (1974).
(X8) Ehmann, A., *Carbohydr. Res.*, 34, 99 (1974).
(X9) Einolf, W. N., Fenselau, C., *Biomed. Mass Spectrom.*, 1, 195 (1974).
(X10) Evans, N., Games, D. E., Harwood, J. L., Jackson, A. H., *Biochem. Soc. Trans.*, 2, 1091 (1974).
(X11) Hanfland, P., Egge, H., *Chem. Phys. Lipids*, 15, 243 (1975).
(X12) Hasegawa, K., Suzuki, T., *Lipids*, 8, 631 (1973).
(X13) Hayashi, A., Matsubara, T., Matsuura, F., *Chem. Phys. Lipids*, 14, 102 (1975).
(X14) Kamerling, J. P., Vliegenthart, J. F. G., Versluis, C., Schauer, R., *Carbohydr. Res.*, 41, 7 (1975).
(X15) Kamerling, J. P., Vliegenthart, J. F. G., Vink, J., *Carbohydr. Res.*, 33, 297 (1974).
(X16) Karlander, S.-G., Karlsson, K. A., Pascher, I., *Biochim. Biophys. Acta*, 326, 174 (1973).
(X17) Karlsson, K.-A., *Biochemistry*, 13, 3643 (1974).
(X18) Karlsson, K.-A., Leffler, H., Samuelsson, B. E., *J. Biol. Chem.*, 249, 4819 (1974).
(X19) Karlsson, K.-A., Pascher, I., Pimlott, W., Samuelsson, B. E., *Biomed. Mass Spectrom.*, 1, 49 (1974).
(X20) Karlsson, K.-A., Pascher, I., Samuelsson, B. E., *Chem. Phys. Lipids*, 12, 271 (1974).
(X21) Karlsson, K.-A., Samuelsson, B. E., *Biochim. Biophys. Acta*, 337, 204 (1974).
(X22) Karlsson, K.-A., Samuelsson, B. E., Steen, G. O., *Biochim. Biophys. Acta*, 337, 358 (1974).
(X23) Karlsson, K.-A., Samuelsson, B. E., Steen, G. O., *Biochim. Biophys. Acta*, 316, 336 (1973).
(X24) Kochetkov, N. K., Sviridov, A. F., Vecherko, L. P., Kadentsev, V. I., Chizhov, O. S., *Bull. Acad. Sci., Div. Chem. Sci.*, 23, 105 (1974); translated from *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1, 113 (1974).
(X25) Komori, T., Ida, Y., Mutou, Y., Miyahara, K., Nohara, T., Kawasaki, T., *Biomed. Mass Spectrom.*, 2, 65 (1975).
(X26) Komori, T., Tanaka, O., Nagai, Y., *Org. Mass. Spectrom.*, 9, 744 (1974)
(X27) Krisnangkura, K., Sweeley, C. C., *Chem. Phys. Lipids*, 13, 415 (1974).
(X28) Ladeen, R. W., Kundu, S. K., Price, H. C., Fong, J. W., *Chem. Phys. Lipids*, 13, 429 (1974).
(X29) Markey, S. P., Wenger, D. A., *Chem. Phys. Lipids*, 12, 182 (1974).
(X30) Ohnishi, M., Nakano, M., Fujino, Y., *Agric. Biol. Chem.*, 39, 743 (1975).
(X31) Prokazova, N. V., Todriya, K. G., Vaver, V. A., Bergel'son, L. D., *Bull. Acad. Sci. USSR, Div. Chem. Sci.*, 23, 2476 (1975); translated from *Izv. akad. Nauk SSSR, Ser. Khim.*, 11, 2569 (1974).
(X32) Schmitz, F. J., McDonald, F. J., *J. Lipid Res.*, 15, 158 (1974).
(X33) Schulten, H.-R., Games, D. E., *Biomed. Mass Spectrom.*, 1, 120 (1974).
(X34) Smith, E. L., McKibbin, J. M., Karlsson, K.-A., Pascher, I., Samuelsson, B. E., *Biochemistry*, 14, 2120 (1975).
(X35) Smith, E. L., McKibbin, J. M., Karlsson, K.-A., Pascher, I., Samuelsson, B. E., *Biochim. Biophys. Acta*, 388, 171 (1975).
(X36) Stellner, K., Hakomori, S. I., *J. Biol. Chem.*, 249, 1022 (1974).
(X37) Viswanathan, C. W., *J. Chromatogr.*, 98, 105 (1974).
(X38) Wagner, H., Seligmann, O., *Tetrahedron*, 29, 3029 (1973), in German.
(X39) Watanabe, K., Laine, R. A., Hakomori, S., *Biochemistry*, 14, 2725 (1975).
(X40) Wood, G. W., Lau, P.-Y., *Biomed. Mass Spectrom.*, 1, 154 (1974).
(X41) Wood, G. W., Lau, P.-Y., Teubner, J., presented at the 22nd Annual Conference on Mass Spectrometry and Allied Topics, Philadelphia, Pa., May 1974, p 273.

**Prostaglandins**

(Y1) Cory, H. T., Lascelles, P. T., Millard, B. J., Sneddon, W., Wilson, B., *Biochem. Soc. Trans.*, 3, 536 (1975).
(Y2) Crain, P. F., Desiderio, D. M., Jr., McCloskey, J. A., in "Methods in Enzymology", Vol. XXXV, J. M. Lowenstein, Ed., Academic Press, New York, 1975, p 359.
(Y3) Danon, A., Chang, L. C. T., Sweetman, B. J., Nies, A. S., Oates, J. A., *Biochim. Biophys. Acta*, 388, 71 (1975).
(Y4) Downie, J., Poyser, N. L., Wunderlich, M., *J. Physiol.*, 238, 465 (1974).
(Y5) Frolich, J. C., Sweetman, B. J., Carr, K., Hollifield, J. W., Oates, J. A., *Prostaglandins*, 10, 185 (1975).
(Y6) Frolich, J. C., Sweetman, B. J., Carr, K., Watson, J. T., Oates, J., *Clin. Res.*, 23, 35A (1974).
(Y7) Frolich, J. C., Williams, W. M., Sweetman, B. J., Smigel, M., Carr, K., Hollifield, J. W., Fleischer, S., Nies, A. S., Frisk-Holmberg, M., Oates, J. A., in "Advances in Prostaglandin and Thromboxane Research", Vol. 1, B. Samuelsson and R. Paoletti, Ed., Raven Press, New York, 1975.
(Y8) Green, K., Bygdeman, M., Toppozada, M., Wiqvist, N., *Am. J. Obstet. Gynecol.*, 120, 25 (1974).
(Y9) Green, K., Hagenfeldt, K., *Am. J. Obstet. Gynecol.*, 122, 611 (1975).
(Y10) Green, K., Hamberg, M., Samuelsson, B., in "Advances in Prostaglandin and Thromboxane Research", Vol. 1, B. Samuelsson and R. Paoletti, Ed., Raven Press, New York, 1975, p 47.
(Y11) Hamberg, M., *Life Sci.*, 14, 247 (1974).
(Y12) Hamberg, M., Samuelsson, B., *Biochem. Biophys. Res. Commun.*, 61, 942 (1974).
(Y13) Hamberg, M., Samuelsson, B., *Proc. Nat. Acad. Sci.*, 71, 3400 (1974).
(Y14) Hamberg, M., Svensson, J., Samuelsson, B., *Proc. Natl Acad. Sci. U.S.A.*, 71, 3824 (1974).
(Y15) Hamberg, M., Svensson, J., Wakabayashi, T., Samuelsson, B., *Proc. Natl. Acad. Sci. U.S.A.*, 71, 345 (1974).
(Y16) Horvath, G., *Biomed. Mass Spectrom.*, 3, in press, 1976.
(Y17) Horvath, G., *Biomed. Mass Spectrom.*, 2, 190 (1975).
(Y18) Jonsson, H. T., Jr., Middleditch, B. S., Desiderio, D. M., *Science*, 187, 1093 (1975).
(Y19) Lee, M. G., Millard, B. J., *Biomed. Mass Spectrom.*, 2, 78 (1975).
(Y20) Middleditch, B. S., Desiderio, D. M., *Adv. Mass Spectrom.*, 6, 173 (1974).
(Y21) Nicosia, S., Galli, G., in "Advances in Prostaglandin and Thromboxane Research", Vol. 1, B. Samuelsson and R. Paoletti, Ed., Raven Press, New York, 1975.
(Y22) Nicosia, S., Galli, G., *Anal. Biochem.*, 61, 192 (1974)
(Y23) Nicosia, S., Galli, G., *Prostaglandins*, 9, 397 (1975).
(Y24) Oswald, E. O., Parks, D., Eling, T., Corbett, B. J., *J. Chromatogr.*, 93, 47 (1974).
(Y25) Samuelsson, B., Granstrom, E., Green, K., Hamburg, M., Hammarström, S., *Ann. Rev. Biochem.*, 44, 669 (1975).
(Y26) Samuelsson, B., Green, K., *Biochem. Med.*, 11, 298 (1974).
(Y27) Seyberth, H. W., Segre, G. V., Morgan, J. L., Sweetman, B. J., Potts, J. T., Jr., Oates, J. A., *N. Engl. J. Med.*, 293, 1278 (1975).
(Y28) Sun, F. F., *Biochim. Biophys. Acta*, 348, 249 (1974).
(Y29) Svensson, J., Hamberg, M., Samuelsson, B., *Acta Physiol. Scand.*, 94, 222 (1975).
(Y30) Taylor, P. L., Kelly, R. W., *FEBS Lett.*, 57, 22 (1975).
(Y31) Taylor, P. L., Kelly, R. W., *Nature (London)*, 250, 665 (1974).
(Y32) Tobias, L. D., Vane, F. M., Paulsrud, J. R., *Prostaglandins*, 10, 443 (1975).
(Y33) Watson, J. T., Sweetman, B. J., *Org. Mass Spectrom.*, 9, 39 (1974).

**Biomedicine and Clinical Chemistry**

(Z1) Abramson, F. P., McCaman, M. W., McCaman, R. E., *Anal. Biochem.*, 61, 482 (1974).
(Z2) Adlercreutz, H., Martin, F., Wahlroos, O., Soini, E., *J. Steroid Biochem.*, 6, 247 (1975).
(Z3) Adlercreutz, H., Soltmann, B., Tikkanen, M. J., *J. Steroid Biochem.*, 5, 163 (1974).
(Z4) Adlercreutz, H., Tikkanen, M. J., Hunneman, D. H., *J. Steroid Biochem.*, 5, 211 (1974).
(Z5) Axelson, M., Schumacher, G., Sjövall, J., *J. Chromatogr. Sci.*, 12, 535 (1974).
(Z6) Axelson, M., Sjövall, J., *J. Steroid Biochem.*, 5, 733 (1974).
(Z7) Back, P., Sjövall, J., Sjövall, K., *Med. Biol.*, 52, 31 (1974).
(Z8) Ballantine, J. A., Roberts, J. C., Morris, R. J., *J. Chromatogr.*, 103, 289 (1975).
(Z9) Baty, J. D., Wade, A. P., *Anal. Biochem.*, 67, 27 (1974).
(Z10) Bègue, R. J., Desgrès, J., Padieu, P. Gustafsson, J. A., *J. Chromatogr. Sci.*, 12, 763 (1974).
(Z11) Björkhem, I., Blomstrand, R., Lantto, O., Löf, A., Svensson, L., *Clin. Chim. Acta*, 56, 241 (1974).
(Z12) Björkhem, I., Blomstrand, R., Svensson, L., *Clin. Chim. Acta*, 54, 185 (1974).
(Z13) Björkhem, I., Blomstrand, R., Svensson, L., Tietz, F., Caristrom, K., *Clin. Chim. Acta*, 62, 385 (1975).
(Z14) Brasellon, W. E., Jr., Orr, J. C., Engel, L. L., *Steroids*, 24, (1974).
(Z15) Brock, A., Heilskov, N. S. C., Kelding, R., Munck, O., Nielsen, A. B., Ed., Trans. XV Meeting of Scandinavian Society for Clinical Chemistry and Clinical Physiology, *Scand. J. Clin. Lab. Invest.*, 35, Suppl. 143 (1975).
(Z16) Byrd, D. J., Kochen, W., Idzko, D., Knorr, E., *J. Chromatogr.*, 94, 85 (1974).
(Z17) Chalmers, R. A., Lawson, A. M., Watts, R. W. E., *Clin. Chim. Acta*, 52, 43 (1974).
(Z18) Chalmers, R. A., Lawson, A. M., *Chem. Br.*, 11, 290 (1975).
(Z19) Chalmers, R. A., Watts, R. W. E., *Clin. Chim. Acta*, 55, 281 (1974).
(Z20) Chapman, J. R., Bailey, E., *J. Chromatogr.*, 89, 215 (1974).
(Z21) Christiansen, P., *Chromatographia*, 8, 463 (1975).
(Z22) Curtius, H. Ch., Wolfensberger, M., Redweik, U., Leimbacher, W., Malbach, R. A., Isler, W., *J. Chromatogr.*, 112, 523 (1975).
(Z23) Dehennin, L., Reiffsteck, A., Scholler, R., *J. Steroid Biochem.*, 5, 767 (1974).
(Z24) De Jongh, D. C., Hills, E. B., *Biomed. Mass Spectrom.*, 2, 117 (1975).
(Z25) Donike, M., *Chromatographia*, 7, 651 (1974).
(Z26) Dowty, B., Carlisle, D., Laseter, J. L., Gonzalez, F. M., *Biomed. Mass Spectrom.*, 2, 142 (1975).
(Z27) Duncan, J. H., Couch, M. W., Gotthelf, G., Scott, K. N., *Biomed. Mass Spectrom.*, 1, 40 (1974).
(Z28) Durden, D. A., Davis, B. A., Boulton, A. A., *Biomed. Mass Spectrom.*, 1, 83 (1974)
(Z29) Eldjarn, L., Jellum, E., Stokke, O., *J.*

*Chromatogr.*, 91, 353 (1974).
(Z30) Eidjarn, L., Jellum, E., Stokke, O., *Clin. Chem.*, 21, 63 (1975).
(Z31) Fales, H. M., Milne, G. W. A., Winkler, H. U., Beckey, H. D., Damico, J. N., Barron, R., *Anal. Chem.*, 47, 207 (1975).
(Z32) Fri, C.-G., Wiesel, F.-A., Sedvall, G., *Life Sci.*, 14, 2469 (1974).
(Z33) Gan, I., Korth, J., Halpern, B., *J. Chromatogr.*, 92, 435 (1974).
(Z34) Gibbs, B. F., Itiaba, K., Crawhall, J. C., *Biochem. Med.*, 11, 165 (1974).
(Z35) Gompertz, D., Saudubray, J. M., Charpentier, C., Bartlett, K., Goodey, P. A., Draffan, G. H., *Clin. Chim. Acta*, 57, 269 (1974).
(Z36) Hanin, I., Skinner, R. F., *Anal. Biochem.*, 66, 568 (1975).
(Z37) Jellum, E., Helland, P., Eidjarn, L., Markwardt, U., Marhöfer, J., *J. Chromatogr.*, 112, 573 (1975).
(Z38) Jelus, B., Munson, B., Fenselau, C., *Anal. Chem.*, 46, 729 (1974).
(Z39) Johnstone, R. A. W., Povall, T. J., Baty, J. D., Pousset, J.-L., Charpentier, C., Lemonnier, A., *Clin. Chim. Acta*, 52, 137 (1974).
(Z40) Karoum, F., Gillin, J. C., Wyatt, R. J., Costa, E., *Biomed. Mass Spectrom.*, 2, 183 (1975).
(Z41) (a) Kimble, B. J., Cox, R. E., McPherron, R. V., Olsen, R. W., Roitman, E., Walls, F. C., Burlingame, A. L., *J. Chromatogr Sci.*, 12, 647 (1974). (b) Kimble, B. J., Cox, R. E., McPherron, R. V., Olsen, R. W., Roitman, E., Walls, F. C., Burlingame, A. L., "Proceedings of the 2nd International Symposium on Mass Spectrometry in Biochemistry and Medicine, Milan, June 1974", A. Frigerio, N. Castagnoli, Ed., Spectrum Publications, New York, in press.
(Z42) Knights, B. A., Legendre, M., Lasater, J. L., Storer, J. S., *Clin. Chem.*, 21, 688 (1975).
(Z43) Lawson, A. M., in "Chemical Biochemistry—Principles and Methods", Vol. II, H. Ch. Curtius and M. Roth, Ed., Walter de Gruyter, Berlin, 1974, p 1653.
(Z44) Lawson, A. M., *Clin. Chem.*, 21, 803 (1975).
(Z45) Lawson, A. M., Chalmers, R. A., Watts, R. W. E., *Biomed. Mass Spectrom.*, 1, 199 (1974).
(Z46) Leclercq, P. A., *Biomed. Mass Spectrom.*, 1, 109 (1974).
(Z47) Lee, M. G., Millard, B. J., *Biomed. Mass Spectrom.*, 2, 78 (1975).
(Z48) Liebich, H. M., *J. Chromatogr.*, 112, 551 (1975).
(Z49) Liebich, H. M., Al-Babbili, O., *J. Chromatogr.*, 112, 539 (1975).
(Z50) Liebich, H. M., Al-Babbili, O., Zlatkis, A., Kim, K., *Clin. Chem.*, 21, 1294 (1975).
(Z51) Lundblad, A., Masson, P. K., Nordén, N. E., Svensson, S., Öckerman, P.-A., *Biomed. Mass Spectrom.*, in press (1976).
(Z52) Mamer, O. A., Mitchell, W. J., Scriver, C. R., Ed., "Application of Gas Chromatography–Mass Spectrometry to the Investigation of Human Disease", McGill University, Montreal Children's Hospital Research Institute, 1974.
(Z53) Mamer, O. A., Tjoa, S. S., *Biomed. Mass Spectrom.*, 2, 133 (1975).
(Z54) Markey, S. P., Urban, W. G., Levine, S. P., "Mass Spectra of Compounds of Biological Interest", Vol. 1 and 2 in collaboration with Committee VI of American Society for Mass Spectrometry, USAEC Technical Information Center, Oak Ridge, Tenn.
(Z55) Maume, B. F., Luyten, J. A., *J. Chromatogr. Sci.*, 2, 607 (1973).
(Z56) Melville, R. S., Dobson, V. F., DHEW Publication #(NIH) 75-782 (1974).
(Z57) Michnowicz, J., Munson, B., *Org. Mass Spectrom.*, 8, 49 (1974).
(Z58) Millington, D. S., *J. Steroid Biochem.*, 6, 239 (1975).
(Z59) Millington, D. S., Bucy, M. E., Brooks, G., Harper, M. E., Griffiths, K., *Biomed. Mass Spectrom.*, 2, 219 (1975).
(Z60) Millington, D., Jenner, D., Jones, T., Griffiths, K., *Biochem. J.*, 139, 473 (1974).
(Z61) Miyazaki, H., Hashimoto, Y., Iwanaga, M., Kubodera, T., *J. Chromatogr.*, 99, 575 (1974).
(Z62) Miyazaki, H., Ishibashi, M., Inoue, M., Itoh, M., Kubodera, T., *J. Chromatogr.*, 99, 553 (1974).
(Z63) Møller, J., With, T. K., *Org. Mass Spectrom.*, 9, 443 (1974).
(Z64) Mrochek, J. E., Rainey, W. T., Jr., *Anal. Biochem.*, 57, 173 (1974).
(Z65) Murata, T., Takahashi, S., Takeda, T., *Anal. Chem.*, 47, 577 (1975)
(Z66) Narasimhachari, N., *J. Chromatogr.*, 90, 183 (1974)
(Z67) Narasimhachari, N., *Biochem. Biophys. Res. Commun.*, 56, 36 (1974)
(Z68) Narasimhachari, N., Lamer, K., Brown, C., *Clin. Chim. Acta*, 62, 245 (1975).
(Z69) Narasimhachari, N., Leuner, K., Plaut, J. M., Lin, R.-L., *Clin. Chim. Acta*, 50, 337 (1974).
(Z70) Nau, H., Biemann, K., *Anal. Chem.*, 46, 426 (1974).
(Z71) Nordén, N. E., Lundblad, A., Svensson, S., Autio, S., *Biochemistry*, 13, 871 (1974).
(Z72) Nyhan, W. L., Ed., "Heritable Disorders of Amino Acid Metabolism", John Wiley & Sons, New York, 1974.
(Z73) Patterson, J. E., *Diabetes*, 23, 16 (1974).
(Z74) Scriver, C. R., Rosenberg, L. E., "Amino Acid Metabolism and Its Disorders", Vol. X, in Major Problems in Clinical Pediatrics series, W. B. Saunders Co., Philadelphia, Pa. 1973.
(Z75) Shackleton, C. H. L., Honour, J. W., *Z. Klin. Chem. Klin. Biochem.*, 8, 25 (1974).
(Z76) Shackleton, C. H. L., Taylor, N. F., *J. Steroid Biochem.*, 6, 1393 (1975).
(Z77) Sjöquist, B., *J. Neurochem.*, 24, 199 (1975).
(Z78) Sjöquist, B., Lindström, B., Änggård, E., *J. Chromatogr.*, 105, 309 (1975).
(Z79) Sjövall, J., *J. Steroid Biochem.*, 6, 227 (1975).
(Z80) Solem, E., Jellum, E., Eidjarn, L., *Clin. Chim. Acta*, 50, 393 (1974).
(Z81) Sweeley, C. C., Young, N. D., Holland, J. F., Gates, S. C., *J. Chromatogr.*, 99, 507 (1974); see also "Proceedings of the 3rd International Symposium on Mass Spectrometry in Biochemistry and Medicine, Sardinia, June 1975", in press.
(Z82) Thompson, J. A., Markey, S. P., *Anal. Chem.*, 47, 1313 (1975).
(Z83) Völkmin, J. A., "Clinical Biochemistry—Principles and Methods", Vol. 1, H. Ch. Curtius and M. Roth, Ed., Walter de Gruyter, Berlin, 1974, p 384.
(Z85) Völkmin, J. A., in "Clinical Biochemistry—Principles and Methods", Vol. 1, H. Ch. Curtius and M. Roth, Ed., Walter de Gruyter, Berlin, 1974, p 753.
(Z85) Wang, M.-T., Imai, K., Yoshioka, M., Tamura, Z., *Clin. Chim. Acta*, 63, 13 (1975).
(Z86) Wang, M.-T., Yoshioka, M., Imai, K., Tamura, Z., *Clin. Chim. Acta*, 63, 21 (1975).
(Z87) Watts, R. W. E., Chalmers, R. A., Lawson, A. M., *Lancet*, I, 368 (1975).
(Z88) Zamboni, F., Blau, K., King, G. S., Campbell, S., Sandler, M., *Clin. Chim. Acta*, 61, 247 (1975).
(Z89) Zeltman, B., Lawless, J. G., *Biochem. Med.*, 13, 111 (1975).
(Z90) Zlatkis, A., Bertsch, W., *J. Chromatogr.*, 91, 379 (1974).

## Pharmacology

(AA1) Agurell, S., Borèus, L. O., Gordon, E., Lindgren, J. E., Ehrnebo, M., Lönroth, U., *J. Pharm. Pharmacol.*, 26, 1 (1974).
(AA2) Baker, K. M., Coerezza, M., Del Corona, L., Frigerio, A., Massaroli, G. G., Sekules, G., *J. Pharm. Sci.*, 63, 293 (1974).
(AA3) Baty, J. D., Price Evans, D. A., Robinson, P. A., *Biomed. Mass Spectrom.*, 1, 128 (1974).
(AA4) Belvedere, G., Burti, L., Frigerio, A., Pantarotto, C., *J. Chromatogr.*, 111, 313 (1975).
(AA5) Belvedere, G., Frigerio, A., Pantarotto, C., *J. Chromatogr.*, 112, 631 (1975).
(AA6) Binder, M., Agurell, S., Leander, K., Lindgren, J.-E., *Helv. Chim. Acta*, 57, 1626 (1974).
(AA7) Björkhem, I., Blomstrand, R., Lantto, O., Svensson, L., *Biochem. Med.*, 12, 205 (1975).
(AA8) Boerner, U., Roe, R. L., Becker, C. E., *J. Pharm. Pharmacol.*, 26, 393 (1974).
(AA9) Bonnichsen, R., Mårde, Y., Ryhage, Y., *Clin. Chem. (Winston-Salem, N.C.)*, 20, 230 (1974).
(AA10) Bourgeois, G., Brachet-Liermain, A., Ferrus, L., *Org. Mass Spectrom.*, 9, 53 (1974).
(AA11) Boyd, P. M., Moses, P. J., Bowman, L., *Spectrosc. Lett.*, 7, 223 (1974).
(AA12) Brent, D. A., de Miranda, P., Schuhen, H.-R., *J. Pharm. Sci.*, 63, 1370 (1974).
(AA13) Breyer, U., Gaertner, H. J., Prox, A., *Biochem. Pharm.*, 23, 313 (1974).
(AA14) Brodasky, T. F., Sun, F. F., *J. Pharm. Sci.*, 63, 360 (1974).
(AA15) Brooks, C. J. W., Gilbert, M. T., *J. Chromatogr.*, 99, 541 (1974).
(AA16) Bulger, W. H., Stohs, S. J., Wheeler, D. M. S., *Biochem Pharm.*, 23, 921 (1974).
(AA17) Chao, J.-M., Saferstein, R., Manura, J., *Anal. Chem.*, 46, 298 (1974).
(AA18) Clarke, P. A., Foltz, R. L., *Clin. Chem. (Winston-Salem, N.C.)*, 20, 485 (1974).
(AA19) Cohen, E. N., Trudell, J. R., Edmunds, H. N., Watson, E., *Anesthesiology*, 43, 392 (1975).
(AA20) Connors, T. A., Cox, P. J., Farmer, P. B., Foster, A. ., Jarman, M., Macleod, J. K., *Biomed Mass Spectrom.*, 1, 130 (1974).
(AA21) Costello, C. E., Hertz, H. S., Sakai, T., Biemann, K., *Clin. Chem (Winston-Salem, N.C.)*, 20, 255 (1974)
(AA22) de Sagher, R. M., de Leenheer, A. P., Claeys, A. E., Cruyl, A. A., *Biomed. Mass Spectrom.*, 2, 82 (1975).
(AA23) Duffield, A. M., in "The Phenothiazines and Structurally Related Drugs", I. S. Forrest, C. J. Carr, E. Usdin, Ed., Raven Press, N.Y., 1974, p 111.
(AA24) Ehrsson, H., *J. Pharm. Pharmacol.*, 27, 971 (1975).
(AA25) Falkner, F. C., Watson, J. T., *Org. Mass Spectrom.*, 8, 257 (1974).
(AA26) Fanelli, R., Frigerio, A., *J. Chromatogr.*, 93, 441 (1974).
(AA27) Faulkner, J. K., Smith, K. J. A., *J. Pharm. Pharmacol.*, 26, 473 (1974).
(AA28) Fenselau, C., Kan, M.-N. N., Billets, S., Colvin, M., *Cancer Res.*, 35, 1453 (1975).
(AA29) Flamm, B. L., Gal, J., *Biomed. Mass Spectrom.*, in press, 1975.
(AA30) Gal, J., Gruenke, L. D., Castagnoli, N., Jr., *J. Med. Chem.*, 18, 683 (1975).
(AA31) Garland, W. A., Trager, W. F., Nelson, S. D., *Biomed. Mass Spectrom.*, 1, 124 (1974).
(AA32) Gilbert, J. N. T., Millard, B. J., Powell, J. W., Straughan, D. W., *Br. J. Pharmacol.*, 47, 665P (1973).
(AA33) Gilbert, J. N., Powell, J. W., *Biomed. Mass Spectrom.*, 1, 142 (1974).
(AA34) Greenwood, H., Snedden, W., Hayward, R. P., Landon, J., *Clin. Chim. Acta*, 62, 213 (1975).
(AA35) Grove, J., Toseland, P. A., Draffan, G. H., Clare, R. A., Williams, F. M., *J. Pharm. Pharmacol.*, 26, 175 (1974).
(AA36) Hansen, A. R., Fischer, L. J., *Clin. Chem. (Winston-Salem, N.C.)*, 20, 236 (1974).
(AA37) Hengstmann, J. H., Falkner, F. C., Watson, J. T., Oates, J., *Anal. Chem.*, 46, 34 (1974).
(AA38) Horning, M. G., Butler, C. M., Nowlin, J., Hill, R. M., *Life Sci.*, 16, 651 (1975).
(AA39) Horning, M. G., Lertratanangkoon, K., Nowlin, J., Stillwell, W. C., Stillwell, R. N., Zlon, T. E., Kellaway, P., Hill, R. M., *J. Chromatogr. Sci.*, 12, 630 (1974).
(AA40) Horning, M. G., Nowlin, J., Butler, C. M., Lertratanangkoon, K., Sommer, K., Hill, R. M., *Clin. Chem. (Winston-Salem, N.C.)*, 21, 1282 (1975).
(AA41) Horning, M. G., Nowlin, J., Stafford, M., Lertratanangkoon, K., Sommer, K. R., Hill, R. M., Stillwell, R. N., *J. Chromatogr.*, 112, 605 (1975).
(AA42) Horning, M. G., Stillwell, W. G., Nowlin, J., Lertratanangkoon, K., Carroll, D., Dzidic, I., Stillwell, R. N. Horning, E. C., *J. Chromatogr.*, 91, 413 (1974).
(AA43) Horning, M. G., Stillwell, W. G., Nowlin, J., Lertratanangkoon, K., Stillwell, R. N., Hill, R. M., *Mod. Probl. Paediatr.*, 15, 73 (1975).
(AA44) Horton, D., Wander, J. D., *Anal. Biochem.*, 59, 452 (1974).
(AA45) Hunneman, D. H., *Chem.-Ztg.*, 98, 28 (1974). In German.
(AA46) Iguchi, S., Goromaru, T., Noda, A., *Chem. Pharm. Bull.*, 23, 932 (1975).
(AA47) Jardine, I., Fenselau, C., *Anal. Chem.*, 47, 730 (1975).
(AA48) Jardine, I., Fenselau, C., *J. Forensic Sci.*, 20, 373 (1975).
(AA49) Jarman, M., Gilby, E. D., Foster, A., Bondy, P. K., *Clin. Chim. Acta*, 58, 61 (1975).
(AA50) Just, W. W., Filipovic, N., Werner, G., *J. Chromatogr.*, 96, 199 (1974).
(AA51) Knight, J. B., Shaikh, M. B., *Anal. Lett.*, 7, 529 (1974).
(AA52) Larsen, N.-E., Naestoft, J., *J. Chromatogr.*, 92, 157 (1974).
(AA53) Lin, D. C. K., Fentiman, A. F., Jr., Foltz, R. L., Forney, R. D., Jr., Sunshine, I., *Biomed. Mass Spectrom.*, 2, 206 (1975).
(AA54) Locock, R. A., Moskalyk, R. E., Chatten, L. G., Lundy, L. M., *J. Pharm Sci.*, 63, 1896 (1974).
(AA55) Marcucci, F., Bianchi, R., Airoldi, L., Saimona, M., Fanelli, R., Chiabrando, C., Frigerio, A., Mussini, E., Garattini, S., *J. Chromatogr.*, 107, 285 (1975).
(AA56) Matin, S. B., Karam, J. H., Forsham, P. H., Knight, J. B., *Biomed. Mass Spectrom.*, 1, 320 (1974)
(AA57) Matin, S. B., Knight, J. B., *Biomed. Mass Spectrom.*, 1, 323 (1974).

(AA58) McReynolds, J. H., Heck, H. d'A., Anbar, M., *Biomed Mass Spectrom.*, in press, 1976.
(AA59) Midha, K. K., *J. Chromatogr.*, 101, 210 (1974).
(AA60) Milberg, R. M., Rinehart, K. L., Jr., Sprague, R. L., Sleator, E. K., *Biomed. Mass Spectrom.*, 2, 2 (1975).
(AA61) Mitscher, L. A., Showalter, H. D. H., Shirahata, K., Foltz, R. L., *J. Antibiot.*, 28, 668 (1975).
(AA62) Miyazaki, H., Ishibashi, M., Izawa, T., Takayama, H., Idzu, G., *Chem. Pharm. Bull.*, 23, 837 (1975).
(AA63) Naestoft, J., Larsen, N.-E., *J. Chromatogr.*, 93, 113 (1974).
(AA64) Nakagawa, T., Masada, M., Uno, T., *J. Chromatogr.*, 111, 355 (1975).
(AA65) Nelson, G. L., Kuhlman, C. F., Chang, T. L., *J. Pharm. Sci.*, 63, 1959 (1974).
(AA66) Pereira, W. E., Summons, R. E., Rindfleisch, T. C., Duffield, A. M., *Clin. Chim. Acta*, 51, 109 (1974).
(AA67) Pfeifer, S., Pöhlmann, H., Kraft, R., *Pharmazie*, 29, 785 (1974), in German.
(AA68) Pohl, L. R., Haddock, R., Garland, W. A., Trager, W. F., *J. Med. Chem.*, 18, 513 (1975).
(AA69) Pohl, L. R., Nelson, S. D., Garland, W. A., Trager, W. F., *Biomed. Mass. Spectrom.*, 2, 23 (1975).
(AA70) Preste, P. G., Westerman, C. E., Das, N. P., Wilder, B. J., Duncan, J. H., *J. Pharm. Sci.*, 63, 467 (1974).
(AA71) Randić, S., Klasinć, L., Šunjic, V., Kajfež, F., Kramer, V., Mildner, P., *Biomed. Mass Spectrom.*, 2, 97 (1975).
(AA72) Rinehart, K. L., Jr., Cook, J. C., Jr., Maurer, K. H., Rapp, U., *J. Antibiot.*, 27, 1 (1974).
(AA73) Rosenfeld, J. J., Bowins, B., Roberts, J., Perkins, J., Macpherson, A. S., *Anal. Chem.*, 46, 2232 (1974).
(AA74) Rouse, D. J., Brent, D. A., *Biomed. Mass Spectrom.*, 1, 256 (1974).
(AA75) Sabih, K., *Biomed. Mass Spectrom.*, 1, 252 (1974).
(AA76) Sabih, K., *Biomed. Mass Spectrom.*, 1, 163 (1974).
(AA77) Sadee, W., Staroscik, J., Finn, C., Cohen, J., *J. Pharm. Sci.*, 64, 998 (1975).
(AA78) Sano, M., Tanaka, Y., *Chem. Pharm. Bull.*, 23, 209 (1975).
(AA79) Schulten, H.-R., *Biomed. Mass Spectrom.*, 1, 223 (1974).
(AA80) Seller, N., Demisch, L., *Biochem. Pharm.*, 23, 259 (1974).
(AA81) Spiteller, G., Remberg, G., *Naturwissenschaften*, 61, 491 (1974), in German.
(AA82) Stillwell, W. G., Stillwell, R. N., Horning, E. C., *Steroids Lipids Res.*, 5, 79 (1974).
(AA83) Sullivan, H. R., Marshall, F. J., McMahon, R. E., Änggård, E., Gunne, L.-M., Holmstrand, J. H., *Biomed. Mass Spectrom.*, 2, 197 (1975).
(AA84) Tatematsu, A., Nadai, L., Yoshizumi, H., *Biomed. Mass Spectrom.*, 1, 66 (1974).
(AA85) Van Boven, M., Janssen, G., Daenens, P., *Mikrochim. Acta*, 603 (1974).
(AA86) Varebely, K., Chedekel, M. A., Mulè, S. J., Rosenthal, D., *Res. Commun. Chem. Pathol. Pharmacol.*, 12, 67 (1975).
(AA87) Wong, L. K., Biemann, K., *Biomed. Mass Spectrom.*, 2, 204 (1975).
(AA88) Wu, A., *Clin. Toxicol.*, 8, 225 (1975).
(AA89) Zak, S. B., Gilleran, T. G., Kartiner, J., Lukas, G., *J. Med. Chem.*, 17, 361 (1974).
(AA90) Zerilli, L. F., Landi, M., Gallo, G. G., Maurer, K. H., Rapp, U., *Biomed. Mass Spectrom.*, in press, 1976.

**Applications in Environmental Chemistry**

(AB1) Alford, A. L., *Biomed. Mass Spectrom.*, 2, 229 (1975).
(AB2) Alford, A. L., *Environ. Prot. Agency Rep.*, No. 660/2-74-002, June 1974.
(AB3) Anders, D. E., Doolittle, F. G., Robinson, W. E., *Geochim. Cosmochim. Acta*, 39, 1423 (1975).
(AB4) Angerer, V. J., Haag, A., Lehnert, G., *Z. Klin. Chem. Biochem.*, 13, 129 (1975).
(AB5) Baughman, R., Meselson, M., *Adv. Chem. Ser.*, 120, 92 (1973).
(AB6) Bergert, K. H., Betz, V., Pruggmayer, D., *Chromatographia*, 7, 115 (1974).
(AB7) Bertsch, W., Anderson, E., Holzer, G., *J. Chromatogr.*, 112, 701 (1975).
(AB8) Bertsch, W., Chang, R. C., Zlatkis, A., *J. Chromatogr. Sci.*, 12, 175 (1974).
(AB9) Bertsch, W., Zlatkis, A., Liebich, H. M., Schneider, H. J., *J. Chromatogr.*, 99, 673 (1974).
(AB10) Blomberg, L., Widmark, G., *J. Chromatogr.*, 106, 59 (1975).
(AB11) Blumer, M., Youngblood, W. W., *Science*, 188, 53 (1975).
(AB12) Boon, J. J., de Leeuw, J. W., Schenk, P. A., in "Advances in Organic Geochemistry 1975", R. Campos, Ed., "Proceedings of the 7th International Meeting for Organic Geochemistry, Madrid, 1975", in press.
(AB13) Boon, J. J., de Leeuw, J. W., Schenk, P. A., *Geochim. Cosmochim. Acta*, 39, 1559 (1975).
(AB14) Boon, J. J., Rijpstra, W. I. C., de Leeuw, J. W., Schenk, P. A., *Nature (London)*, 258, 414 (1975).
(AB15) Boyer, K. W., Laitinen, H. A., *Environ. Sci. Technol.*, 9, 457 (1975).
(AB16) Bruner, F., Brancaleoni, E., *Chim. Ind. (Milan)*, 57, 347 (1975).
(AB17) Budde, W. L., Eichelberger, J. W., "Proceedings of the Symposium on Identification and Analysis of Organic Pollutants in Water, Mexico City, 1975", L. Keith, Ed., in press.
(AB18) Burlingame, A. L., Kimble, B. J., de Leeuw, J. W., Scott, E. S., Wilson, D. M., Stasch, M. J., "Proceedings of the Symposium on Identification and Analysis of Organic Pollutants in Water, Mexico City, 1975", L. Keith, Ed., in press.
(AB19) Burlingame, A. L., Kimble, B. J., Scott, E. S., de Leeuw, J. W., Walls, F. C., "Proceedings of the Symposium on Identification and Analysis of Organic Pollutants in Water, Mexico City, 1975", L. Keith, Ed., in press.
(AB20) Cram, S. P., Juvet, R. S., Jr., Fundamental Review on Gas Chromatography, *Anal. Chem.*, 411 R (1976).
(AB21) Crainwell, P. A., *Chem. Geol.*, 14, 1 (1974).
(AB22) Daun, H., Gilbert, S. G., Glacin, J., *J. Am. Oil Chem. Soc.*, 51, 404 (1974).
(AB23) Didyk, B., Alturki, Y. I. A., Pillinger, C. T., Eglinton, G., *Chem. Geol.*, 15, 193 (1975).
(AB24) Didyk, B. M., Alturki, Y. I. A., Pillinger, C. T., Eglinton, G., *Nature (London)*, 258, 583 (1975).
(AB25) Dougherty, R. C., Roberts, J. D., Biros, F. J., *Anal. Chem.*, 47, 54 (1975).
(AB26) Dowty, B. J., Carlisle, D. R., Laseter, J. L., *Environ. Sci. Technol.*, 9, 762 (1975).
(AB27) Dowty, B., Carlisle, D., Laseter, J. L., Storer, J., *Science*, 187, 75 (1975).
(AB28) Dzidic, I., Carroll, D. I., Stillwell, R. N., Horning, E. C., *Anal. Chem.*, 47, 1308 (1975).
(AB29) Eglinton, G., Sr. Reporter, "Environmental Chemistry", Vol. 1, Specialist Periodical Report, The Chemical Society, London, 1975.
(AB30) Eglinton, G., Firth, J. N. M., Welters, B. L., *Chem. Geol.*, 13, 125 (1974).
(AB31) Eglinton, G., Simoneit, B. R. T., Zoro, J. A., *Proc. R. Soc. London, Ser. B*, 189, 415 (1975).
(AB32) Eichelberger, J. W., Harris, L. E., Budde, W. L., *Anal. Chem.*, 46, 227 (1974).
(AB33) Evans, J. E., Arnold, J. T., *Environ. Sci. Technol.*, 9, 1134 (1975).
(AB34) Evans, K. P., Mathias, A., Mellor, N., Silvester, R., Williams, A. E., *Anal. Chem.*, 47, 821 (1975).
(AB35) Finnigan, R. E., Knight, J. B., "Proceedings of the Symposium on Identification and Analysis of Organic Pollutants in Water, Mexico City, 1975", L. Keith, Ed., in press.
(AB36) Fishbein, L., *J. Chromatogr.*, 99, 177 (1974).
(AB37) Fishbein, L., "Chromatography of Environmental Hazards", Vol. I and II, Elsevier Scientific Publishing, Amsterdam, 1973.
(AB38) Fisher, I. P., Johnson, A., *Anal. Chem.*, 47, 59 (1975).
(AB39) Fisher, I. P., Fischer, P., *Talanta*, 21, 867 (1974).
(AB40) Gallegos, E. J., *Anal. Chem.*, 47, 1150 (1975).
(AB41) Gallegos, E. J., *Anal. Chem.*, 47, 1524 (1975).
(AB42) Gallegos, E. J., Whittemore, I. M., Klaver, R. F., *Anal. Chem.*, 46, 157 (1974).
(AB43) Garty, O. M., Lewis, J. W., Brydia, L. E., *Anal. Chem.*, 46, 815 (1974).
(AB44) Giger, W., Blumer, M., *Anal. Chem.*, 46, 1663 (1974).
(AB45) Giger, W., Reinhard, M., Schaffner, C., *Vom Wasser*, 43, 343 (1974).
(AB46) Glaze, W. H., Henderson, J. E., IV, *J. Water Pollut. Control Fed.*, 47, 2511 (1975).
(AB47) Glaze, W. H., Henderson, J. E., Smith, G., "Proceedings of the Symposium on Identification and Analysis of Organic Pollutants in Water, Mexico City, 1975", L. Keith, Ed., in press.
(AB48) Grimsrud, E. P., Rasmussen, R. A., *Atmos Environ*, 9, 1010 (1975).
(AB49) Grimsrud, E. P., Rasmussen, R. A., *Atmos. Environ.*, 9, 1014 (1975).
(AB50) Grob, R. L., Ed., "Chromatographic Analysis of the Environment", Marcel Dekker, New York, 1975.
(AB51) Hamming, M. C., Redd, F. J., Carel, A. B., "23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975", p 234.
(AB52) Haque, R., Biros, F. J., Ed., "Mass Spectrometry and NMR Spectroscopy in Pesticide Chemistry", Plenum Press, New York, 1974.
(AB53) Harris, L. E., Budde, W. L., Eichelberger, J. W., *Anal. Chem.*, 46, 1912 (1974).
(AB54) Hayatsu, R., Studier, M. H., Moore, L. P., Anders, E., *Geochim. Cosmochim. Acta*, 39, 471 (1975).
(AB55) Heller, S. R., McGuire, J. M., Budde, W. L., *Environ. Sci. Technol.*, 9, 210 (1975).
(AB56) Herlan, A., *Erdoel. Kohle, Erdgas, Petrochem. Brennst.-Chem.*, 27, 138 (1974).
(AB57) Hertz, H. S., May, W. E., Chesler, S. N., Gump, B. H., "23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975", p 663.
(AB58) Hirota, H., Moriyama, Y., Tsuyuki, T., Tanahashi, Y., Takahashi, T., Katoh, Y., Satoh, H., *Bull. Chem. Soc. Jpn*, 48, 1884 (1975).
(AB59) Holmstead, R. L., Casida, J. E., *J. Assoc. Offic. Anal. Chem.*, 58, 541 (1975).
(AB60) Holmstead, R. L., Casida, J. E., *J. Assoc. Offic. Anal. Chem.*, 57, 1050 (1974).
(AB61) Holmstead, R. L., Khalifa, S., Casida, J. E., *J. Agric. Food Chem.*, 22, 939 (1974).
(AB62) Hoyland, J. R., Neher, M. B., *Environ. Prot. Agency Rep.*, EPA-660/2-74-048, June 1974.
(AB63) Hrutfiord, B. F., Friberg, T. S., Wilson, D. F., Wilson, J. R., *Environ. Prot. Agency Rep.*, EPA-660/2-75-028, June 1975.
(AB64) Huertas, M. L., Marty, A. M., Fontan, J., *J. Geophys. Res.*, 79, 1737 (1974).
(AB65) Hutzinger, O., Jamieson, W. D., Safe, S., Paulmann, L., Ammon, R., *Nature (London)*, 252, 698 (1974).
(AB66) Ishiwatari, R., Hanya, T., in "Advances in Organic Geochemistry 1973", B. Tissot and F. Bienner, Ed., Éditions Technip, Paris, p 1051.
(AB67) Jaeger, R. J., Hites, R. A., *Bull. Environ. Contam. Toxicol.*, 11, 45 (1974).
(AB68) Junghans, R. C., Ed., "Marine Pollution Monitoring (Petroleum)", Proc. Symposium and Workshop at National Bureau of Standards, Gaithersburg, Md., May 1974, *Nat. Bur. Stand. (U.S.A.) Spec. Publ.*, 409, 1974.
(AB69) Junk, G. A., "Organics in Drinking Water. Part II. Mass Spectral Identification Data", National Technical Information Service, *Rep.* IS-3672, 1975.
(AB70) Junk, G. A., Svec, H. J., Vick, R. D., Avery, M. J., *Environ. Sci. Technol.*, 8, 1100 (1974).
(AB71) Karasek, F. W., Kim, S. H., *Anal. Chem.*, 47, 1166 (1975).
(AB72) Karasek, F. W., Smythe, R. J., Laub, R. J., *J. Chromatogr.*, 101, 125 (1974).
(AB73) Keith, L. H., *Environ. Prot. Agency Rep.*, EPA-660/4-75-005, June 1975.
(AB74) Keith, L. H., *Sci. Total Environ.*, 3, 87 (1974).
(AB75) Keith, L. H., Garrison, A. W., Allen, F. R., Carter, M. H., Floyd, T. L., Pope, J. D., Thruston, A. D., Jr., "Proceedings of the Symposium on Identification and Analysis of Organic Pollutants in Water, Mexico City, 1975", in press.
(AB76) Kikuchi, T., Mimura, T., Masada, Y., Inoue, T., *Chem. Pharm. Bull.*, 21, 1847 (1973).
(AB77) Kimble, B. J., Maxwell, J. R., Philp, R. P., Eglinton, G., *Chem. Geol.*, 14, 173 (1974).
(AB78) Kimble, B. J., Maxwell, J. R., Philp, R. P., Eglinton, G., Albrecht, P., Ensminger, A., Arpino, R., Ourisson, G., *Geochim. Cosmochim. Acta*, 38, 1165 (1974).
(AB79) Lao, R. C., Thomas, R. S., Monkman, J. L., *J. Chromatogr.*, 112, 681 (1975).
(AB80) Ladet, E. J., Laseter, J. L., *Science*, 186, 261 (1974).
(AB81) Lumpkin, H. E., Elliott, R. M., Evans, S., Hazelby, D., Wolstenholme, W. A., "23rd Annual Conference on Mass Spectrometry and Allied Topics, Houston, Texas, 1975", p 235.
(AB82) Manka, J., Rebhun, M., Mandelbaum, A., Bortinger, A., *Environ Sci. Technol.*, 8, 1017 (1974).
(AB83) McGuire, J. M., Alford, A. L., Carter, M. H., *Environ. Prot. Technol. Ser.*, EPA-R2-73-234, July 1973.
(AB84) McMahon, D. H., Crowell, E. P., *J. Am. Oil*

*Chem. Soc.*, 51, 522 (1974).
(AB85) Ogura, K., *Jap. J. Limnol.*, 34, 129 (1973).
(AB86) Ogura, K., Hanya, T., *Mass Spectrosc.*, 22, 281 (1974).
(AB87) Campos, R., Ed., "Advances in Organic Geochemistry 1975", Proceedings of the 7th International Meeting on Organic Geochemistry, Madrid, 1975, in press.
(AB88) Oswald, E. O., Albro, P. W., McKinney, J. D., *J. Chromatogr.*, 98, 363 (1974).
(AB89) Oswald, E. O., Levy, L., Corbett, B. J., Walker, M. P., *J. Chromatogr.*, 93, 63 (1974).
(AB90) Pedersen, K. R., Lam, J., *Groenl. Geol. Unders., Bull.*, 5 (1975).
(AB91) Pereira, W. E., Summons, R. E., Rindfleisch, T. C., Duffield, A. M., Zeitman, B., Lawless, J. G., *Geochim Cosmochim. Acta*, 38, 1631 (1975).
(AB92) Perry, R., Twibell, J. D., *Biomed. Mass Spectrom.*, 1, 73 (1974).
(AB93) Pierce, R. C., Katz, M., *Environ. Sci. Technol.*, 10, 45 (1976).
(AB94) Pitt, W. W., Jolley, R. L., Katz, S., *Environ. Prot. Agency Rep.*, EPA-660/2-74-076, August 1974.
(AB95) Price, P., Martinsen, D. P., Upham, R. A., Swofford, H. S., Jr., Buttrill, S. E., Jr., *Anal. Chem.*, 47, 190 (1975).
(AB96) Rasmussen, D. V., *Anal. Chem.*, 48, 602 (1974).
(AB97) Reinard, M., Drevenkar, V., Giger, W., *J. Chromatogr.*, 116, 43 (1975).
(AB98) Reynolds, W. D., Delongchamp, R., *Biomed Mass Spectrum.*, 2, 276 (1975).
(AB99) Rook, J. J., *Water Treat. Exam.*, 23, 234 (1974).
(AB100) Rosen, J. D., Morano, J. R., Pareles, S. R., Glacin, J. R., Gilbert, S. G., *J. Am. Offic. Anal. Chem.*, 58, 700 (1975)
(AB101) Rubinstein, I., Sieskind, O., Albrecht, P., *J. Chem. Soc., Perkin Trans. 1*, 1833 (1975).
(AB102) Ruzicka, J. H. A., Abbott, D. C., *Talanta*, 20, 1261 (1973).
(AB103) Safe, S., Jamieson, W. D., Hutzinger, O., Pohland, A. E., *Anal. Chem.*, 47, 327 (1975).
(AB104) Safe, S., Platonow, N., Hutzinger, O., Jamieson, W. D., *Biomed. Mass Spectrom.*, 2, 201 (1975).
(AB105) Scheiman, M. A., Saunders, R. A., Saalfeld, F. E., *Biomed. Mass Spectrom.*, 1, 209 (1974).
(AB106) Schnitzer, M., Skinner, S. I. M., *Can. J. Chem.*, 52, 1072 (1974).
(AB107) Schuetzle, D., *Biomed. Mass Spectrom.*, 3, 131 (1976), in press.
(AB108) Schulten, H. R., Schurath, U., *J. Phys. Chem.*, 79, 51 (1975).
(AB109) Schultz, J. L., Sharkey, A. G., Jr., Friedel, R. A., Nathanson, B., *Biomed. Mass Spectrom.*, 1, 137 (1974).
(AB110) Seifert, W. K., *Prog. Chem. Org. Nat. Prod.*, 32, 1 (1975).
(AB111) Sigmond, T., *Vacuum*, 25, 239 (1975).
(AB112) Skinner, S. I. M., Schnitzer, M., *Anal. Chim Acta*, 75, 207 (1975).
(AB113) Swansiger, J. T., Dickson, F. E., Best, H. T., *Anal. Chem.*, 46, 730 (1974).
(AB114) Tennakoon, D. T. B., Thomas, J. M., Tricker, M. J., Graham, S. H., *J. Chem. Soc., Chem. Commun.*, 124 (1974).
(AB115) Tissot, B., Blenner, F., Ed., "Advances in Organic Geochemistry 1973", Editions Technip, Paris, 1974.
(AB116) Tricker, M. J., Tennakoon, D. T. B., Thomas, J. M., Heald, J., *Clays Clay Miner.*, 23, 77 (1975).
(AB117) Tyson, B. J., Carle, G. C., *Anal. Chem.*, 46, 610 (1974).
(AB118) van Dorsselaer, A., Ensminger, A., Spyckerelle, C., Dastillung, M., Sieskind, O., Arpino, P., Albrecht, P., Ourisson, G., Brooks, P. W., Gaskell, S. J., Kimble, B. J., Philp, R. P., Maxwell, J. R., Eglinton, G., *Tetrahedron Lett.*, 1349 (1974).
(AB119) Webb, R. G., *Environ. Prot. Agency Rep.*, 660/4-75-003, June 1975.
(AB120) Webb, R. G., Garrison, A. W., Keith, L. H., McGuire, J. M., *Gov. Rep. Announce. (USA)*, 74, 57 (1974).
(AB121) Williams, D. T., Miles, W. F., *J. Assoc. Offic. Anal. Chem.*, 58, 272 (1975).
(AB122) Youngblood, W. W., Blumer, M., *Geochim. Cosmochim. Acta*, 39, 1303 (1975).